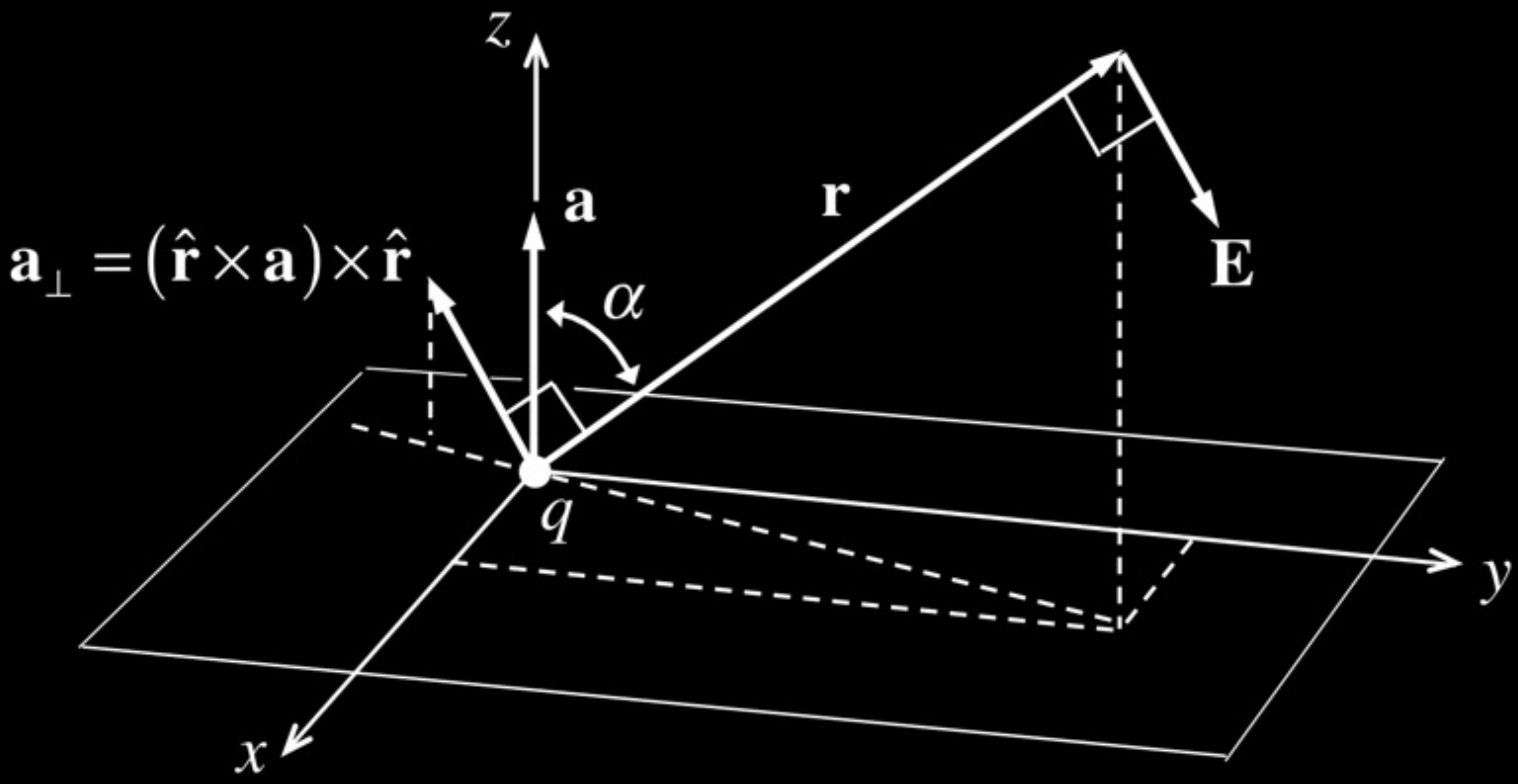
X-Ray scattering by a…

- free electron at rest
- bound electron in a free atom with $\omega >> \omega_0$
- bound electron in a free atom with $\omega \approx \omega_0$
- many-electron atom
- polyatomic molecule
- lattice row
- crystal structure

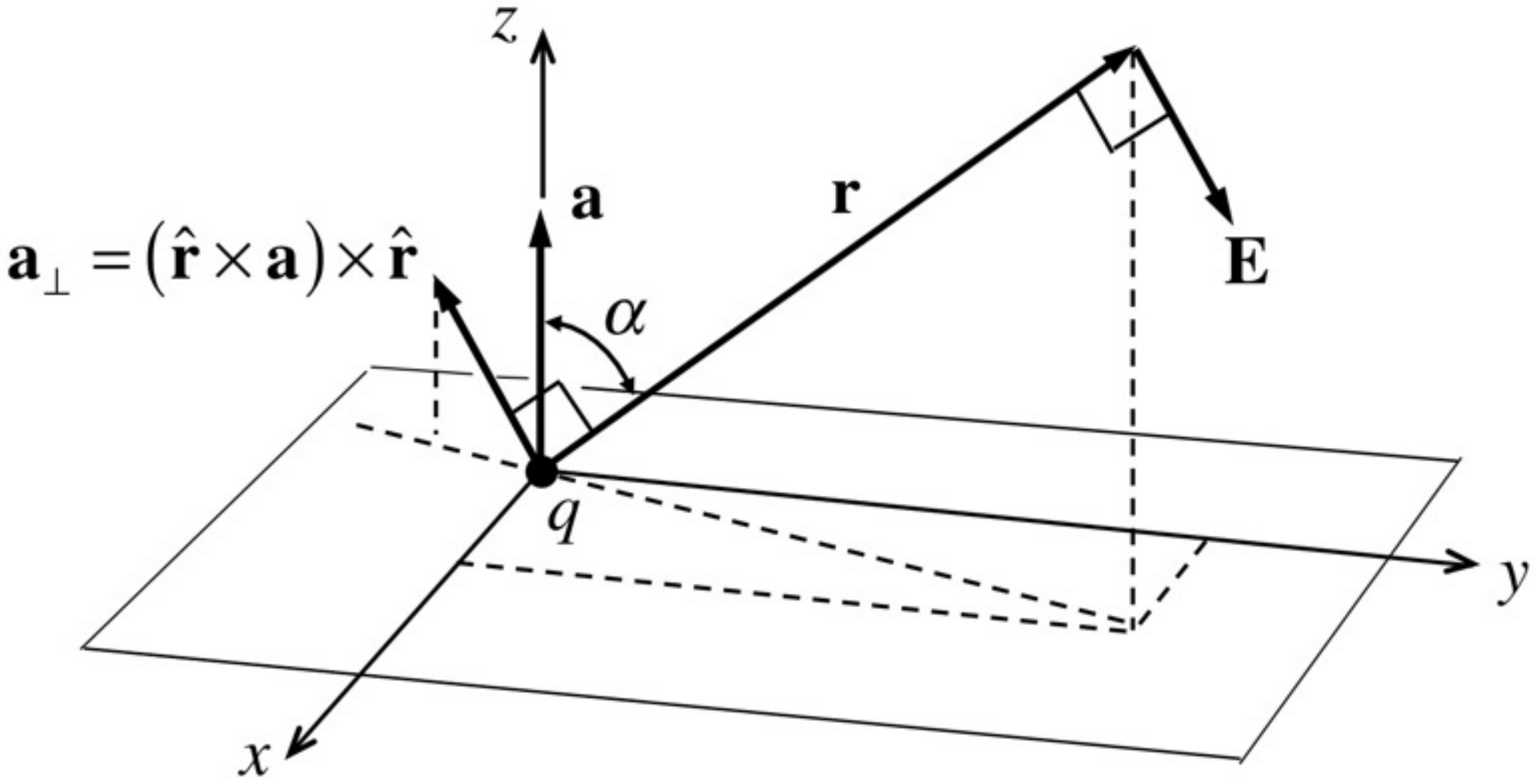
Electric field **E** at a point at **r** from a charge **q** that experiences an acceleration **a**



$$\mathbf{E} = -\frac{q}{c^2 r}(\hat{\mathbf{r}} \times \mathbf{a}) \times \hat{\mathbf{r}}, \qquad \hat{\mathbf{r}} = \frac{\mathbf{r}}{|\mathbf{r}|}, \qquad |\mathbf{r}| = r$$

$$E = -\frac{q}{c^2 r} a \sin\alpha, \qquad E = |\mathbf{E}|, \qquad a = |\mathbf{a}|$$

Electric field **E** at a point at **r** from a charge **q** that experiences an acceleration **a**



$$\mathbf{E} = -\frac{q}{c^2 r}(\hat{\mathbf{r}} \times \mathbf{a}) \times \hat{\mathbf{r}} \,, \qquad \hat{\mathbf{r}} = \frac{\mathbf{r}}{|\mathbf{r}|} \,, \qquad |\mathbf{r}| = r$$

$$E = -\frac{q}{c^2 r} a \sin\alpha \,, \qquad E = |\mathbf{E}| \,, \qquad a = |\mathbf{a}|$$

X-ray scattering by a free electron at rest (Gaussian cgs units)

driven harmonic oscillator

Coulombic em driving force

$$\mathbf{F} = q\mathbf{E} = q_{\mathrm{e}}\mathbf{E} = -e\,\underbrace{\mathbf{E}_0\,\mathrm{e}^{i\omega t}}_{\text{incident X-ray plane wave}} = -e\,\mathbf{E}_0\left[\cos(\omega t) + i\sin(\omega t)\right]$$

Newton's second law of motion

$$\mathbf{F} = m\mathbf{a} = m_{\mathrm{e}}\,\frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2}$$

$$m\,\mathbf{a} = q\mathbf{E}$$

$$m_{\mathrm{e}}\mathbf{a} = -e\mathbf{E}_0\,\mathrm{e}^{i\omega t}$$

$$\mathbf{a} = \frac{-e\mathbf{E}_0}{m_{\mathrm{e}}}\mathrm{e}^{i\omega t} = \mathbf{a}_0\,\mathrm{e}^{i\omega t}, \qquad \mathbf{a}_0 = \frac{-e\mathbf{E}_0}{m_{\mathrm{e}}}$$

em radiation from an accelerated charge

$$\mathcal{E} = -\frac{q}{c^2 r}\mathbf{a}_{\perp}, \qquad |\mathcal{E}| = -\frac{q}{c^2 r}|\mathbf{a}|\sin\alpha, \qquad \alpha = \measuredangle\,\mathbf{a},\mathbf{r}$$

$$\mathcal{E} = -\frac{q}{c^2 r}(\hat{\mathbf{r}}\times\mathbf{a})\times\hat{\mathbf{r}} = -\frac{q}{c^2 r}\left(\frac{\mathbf{r}}{r}\times\mathbf{a}\right)\times\frac{\mathbf{r}}{r}$$

$$\mathcal{E}_0 = -\frac{q_{\mathrm{e}}}{c^2 r}\,\mathbf{a}_0 = -\frac{-e}{c^2 r}\left(\frac{-e\mathbf{E}_0}{m_{\mathrm{e}}}\right) = -\underbrace{\left(\frac{e^2}{m_{\mathrm{e}}c^2}\right)\frac{\mathbf{E}_0}{r}}_{\text{scattered X-ray spherical wave}} = -r_{\mathrm{e}}\,\frac{\mathbf{E}_0}{r}$$

Amplitude at **r** in the equatorial plane perpendicular to the polarization direction

X-ray scattering by a free electron, at rest or moving uniformly at a nonrelativistic velocity

(Gaussian cgs units)

$$\begin{cases} \mathbf{F}_{\text{Coulomb}} = q\mathbf{E} \\ \mathbf{F}_{\text{Newton}} = m\mathbf{a} \end{cases}$$

$$m\mathbf{a} = -e\,\mathbf{E}_0 \mathrm{e}^{i\omega t}$$

Newton's second law force **F=*m*a**

em Coulombic driving force **F=*q*E**

$$\mathbf{a} = -\frac{e}{m}\mathbf{E}_0 \mathrm{e}^{i\omega t}$$

$$\mathcal{E} = -\frac{q\,\mathbf{a}_\perp}{c^2 r} = -\frac{q}{c^2 r}(\hat{\mathbf{r}} \times \mathbf{a}) \times \hat{\mathbf{r}}\,, \qquad \hat{\mathbf{r}} = \frac{\mathbf{r}}{|\mathbf{r}|}\,, \qquad |\mathcal{E}| = -\frac{q}{c^2 r}|\mathbf{a}|\sin\alpha\,, \qquad \alpha = \measuredangle\,\mathbf{a},\mathbf{r}$$

$$\mathcal{E} = -\frac{q\,\mathbf{a}}{c^2 r} = -\left(\frac{-e}{c^2 r}\right)\left(\frac{-e\mathbf{E}_0}{m}\right)\mathrm{e}^{i\omega t} = \underbrace{-\underbrace{\left(\frac{e^2}{mc^2}\right)}_{\text{Thomson scattering length}}\frac{\mathbf{E}_0}{r}}_{\mathcal{E}_0}\,\mathrm{e}^{i\omega t} = \mathcal{E}_0 \mathrm{e}^{i\omega t}$$

X-ray scattering by a free electron (Gaussian cgs units)

$$\underbrace{\mathcal{E}_0\mathrm{e}^{i\omega t}}_{\substack{\text{scattered}\\ \text{X-ray}\\ \text{wave}}} = -\underbrace{\left(\frac{e^2}{mc^2}\right)}_{\substack{r_\mathrm{e}\\ \text{Thomson}\\ \text{scattering}\\ \text{length}}}\frac{\mathbf{E}_0}{r}\mathrm{e}^{i\omega t} = -r_\mathrm{e}\,\frac{\mathbf{E}_0}{r}\mathrm{e}^{i\omega t} = -\frac{r_\mathrm{e}}{r}\mathbf{E}_0\mathrm{e}^{i\omega t}$$

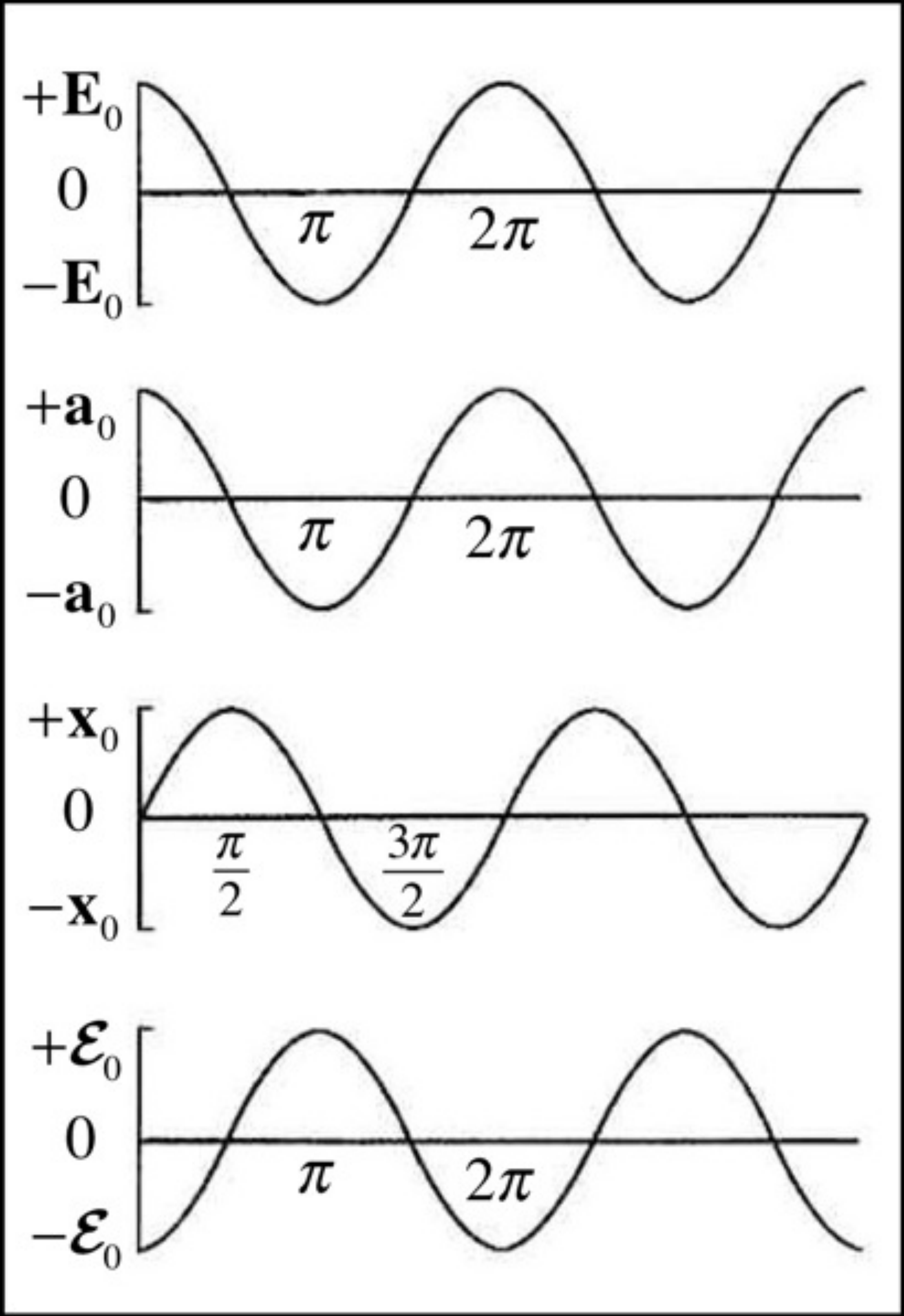
$$r_\mathrm{e} = \underbrace{\left(\frac{e^2}{mc^2}\right)}_{\substack{\text{classical}\\ \text{electron}\\ \text{radius}}}$$

$$\frac{\text{charge}^2}{\text{mass}\bullet\text{velocity}^2} = \frac{\text{charge}^2}{\text{mass}\bullet\text{distance}^2\bullet\text{time}^{-2}} = \frac{\text{force}}{\text{mass}\bullet\text{time}^{-2}} = \frac{\text{acceleration}}{\text{time}^{-2}} = \text{distance}$$

Classical electron radius

$$\left.\begin{array}{l}\text{Electrostatic potential energy}\\ \qquad E = q\phi(r) = q(q/r) = e^2/r_\mathrm{e}\\ \text{Relativistic mass - energy}\\ \qquad E = m_\mathrm{e}c^2\end{array}\right\}\quad r_\mathrm{e} = \frac{e^2}{m_\mathrm{e}c^2}$$

Phase reversal upon scattering of an electromagnetic wave by a point charge



incident em wave

$$\begin{cases} \varphi_{\mathbf{E}} \\ \mathbf{E} = \mathbf{E}_0 e^{i\omega t} \end{cases}$$

charge acceleration

$$\begin{cases} \varphi_{\mathbf{a}} = \varphi_{\mathbf{E}} \\ \mathbf{a} = \mathbf{a}_0 e^{i\omega t} \end{cases}$$

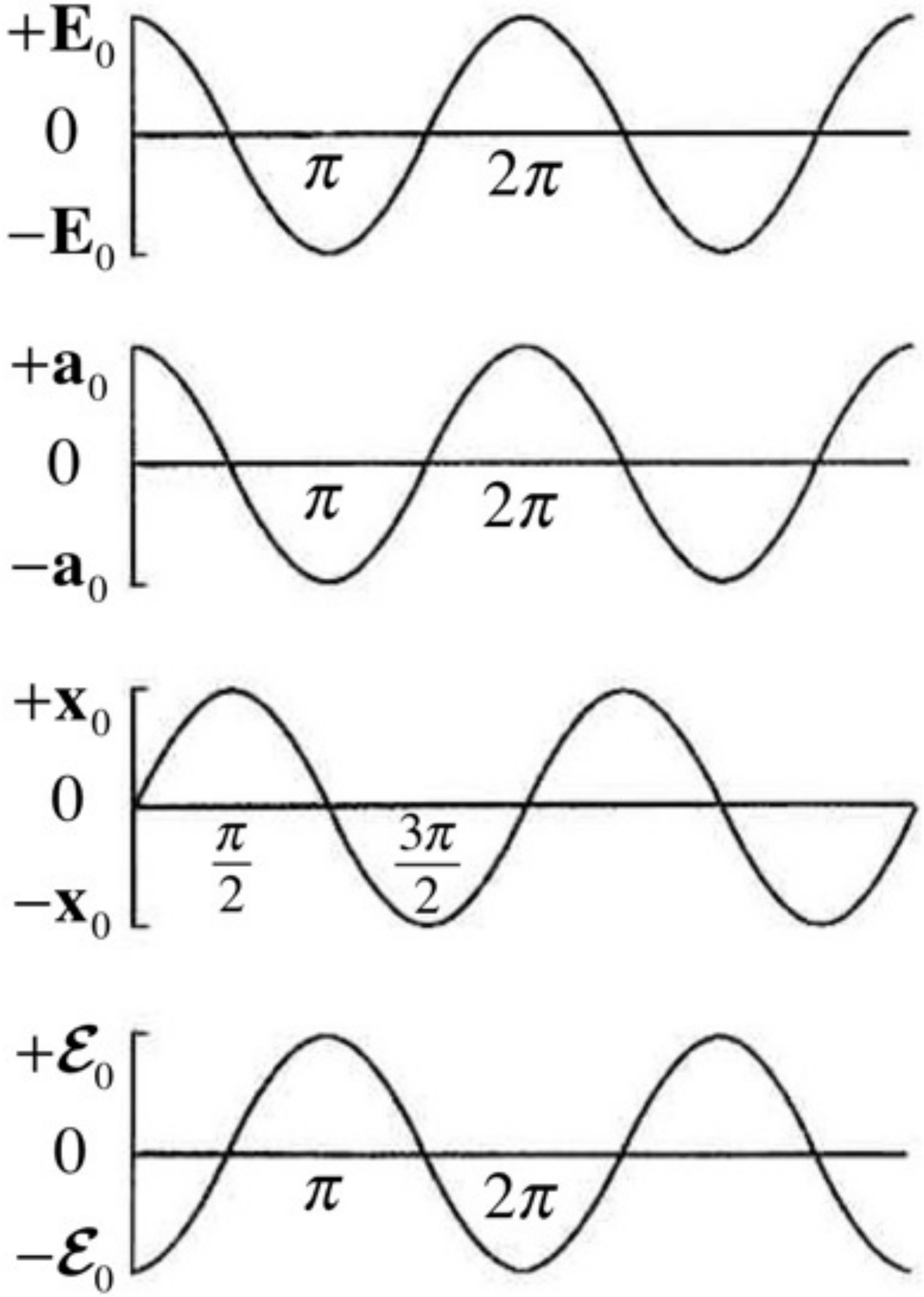
charge displacement

$$\begin{cases} \varphi_{\mathbf{x}} = \left(\varphi_{\mathbf{a}} - \frac{\pi}{2}\right) = \left(\varphi_{\mathbf{E}} - \frac{\pi}{2}\right) \\ \mathbf{x} = \mathbf{x}_0 \exp\left[i\left(\omega t - \frac{\pi}{2}\right)\right] \end{cases}$$

scattered em wave

$$\begin{cases} \varphi_{\mathcal{E}} = \left(\varphi_{\mathbf{x}} - \frac{\pi}{2}\right) = \left(\varphi_{\mathbf{E}} - \pi\right) \\ \mathcal{E} = \mathcal{E}_0 \exp\left[i(\omega t - \pi)\right] \end{cases}$$

Phase reversal upon scattering of an electromagnetic wave by a point charge



incident em wave

$$\begin{cases}\varphi_{\mathbf{E}} \\ \mathbf{E} = \mathbf{E}_0 \mathrm{e}^{i\omega t}\end{cases}$$

charge acceleration

$$\begin{cases}\varphi_{\mathbf{a}} = \varphi_{\mathbf{E}} \\ \mathbf{a} = \mathbf{a}_0 \mathrm{e}^{i\omega t}\end{cases}$$

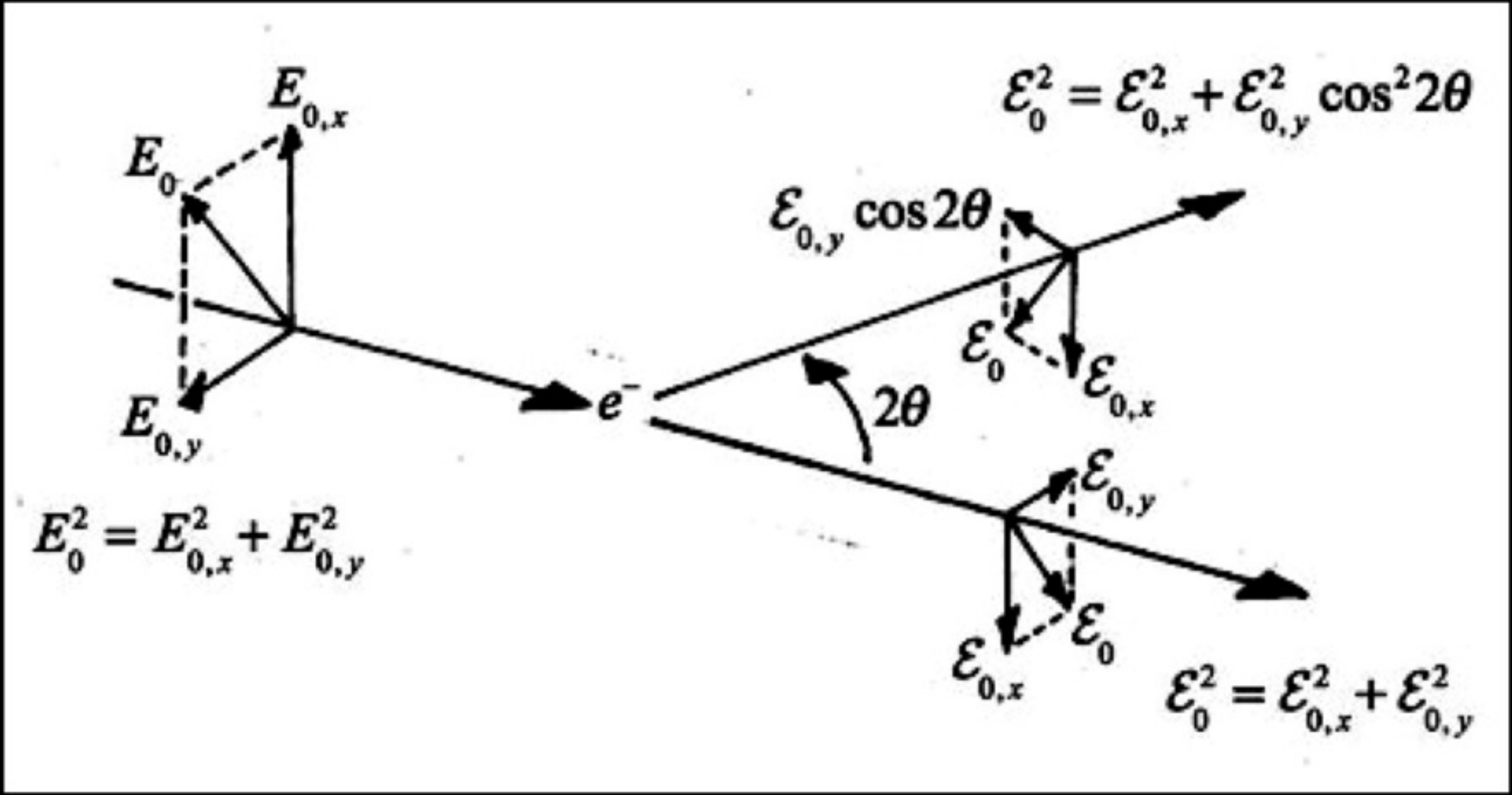
charge displacement

$$\begin{cases}\varphi_{\mathbf{x}} = \left(\varphi_{\mathbf{a}} - \dfrac{\pi}{2}\right) = \left(\varphi_{\mathbf{E}} - \dfrac{\pi}{2}\right) \\ \mathbf{x} = \mathbf{x}_0 \exp\left[i\left(\omega t - \dfrac{\pi}{2}\right)\right]\end{cases}$$

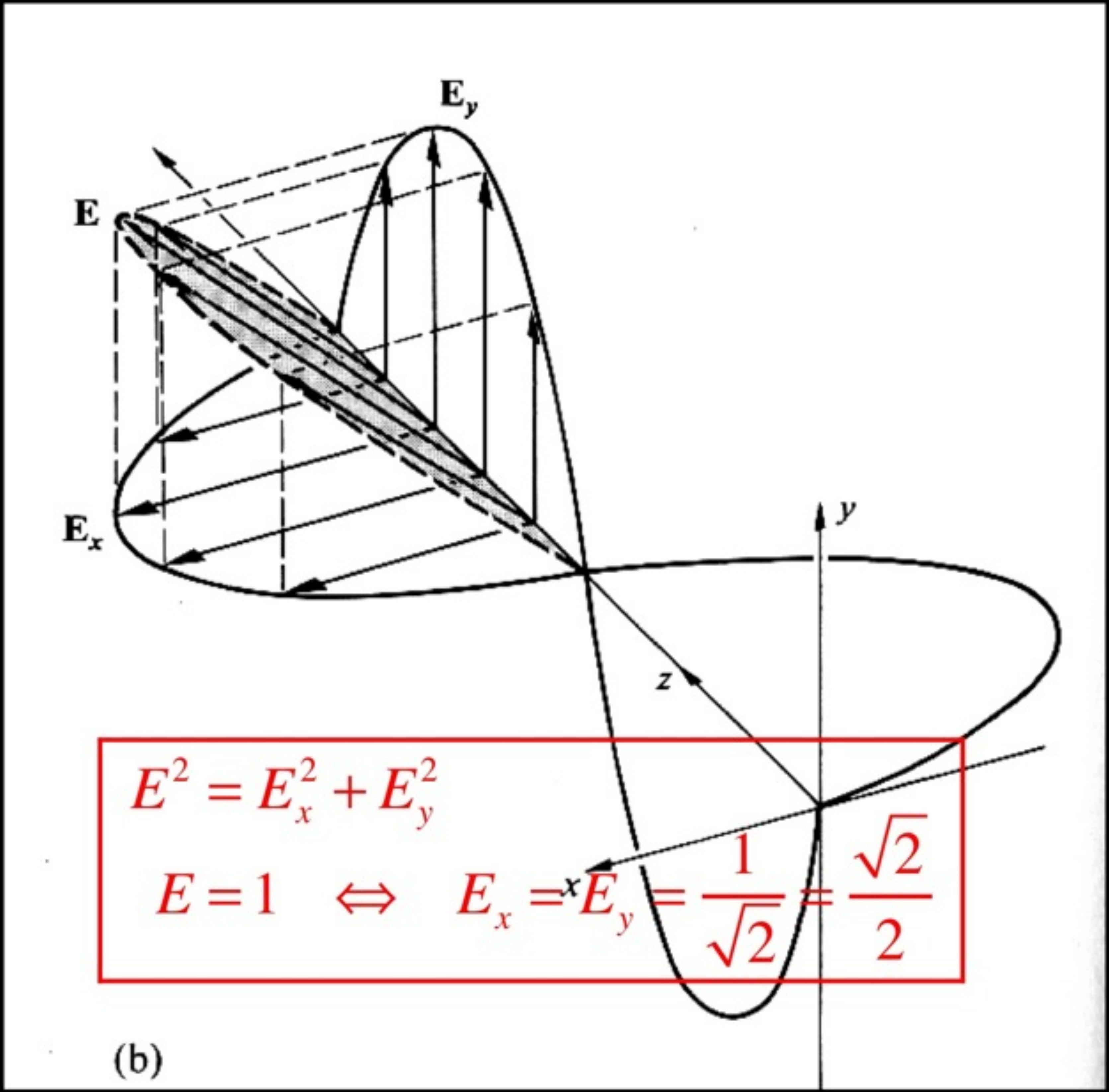
scattered em wave

$$\begin{cases}\varphi_{\mathcal{E}} = \left(\varphi_{\mathbf{x}} - \dfrac{\pi}{2}\right) = \left(\varphi_{\mathbf{E}} - \pi\right) \\ \mathcal{E} = \mathcal{E}_0 \exp\left[i(\omega t - \pi)\right]\end{cases}$$

Scattering of a linearly polarized beam with an arbitrary direction of polarization



Resolved perpendicular components of polarization



$$E^2 = E_x^2 + E_y^2$$

$$E = 1 \quad \Leftrightarrow \quad E_x = E_y = \frac{1}{\sqrt{2}} = \frac{\sqrt{2}}{2}$$

http://www.star.le.ac.uk/~rw/courses/lect4313_fig5.jpg

Scattering of polarized em radiation

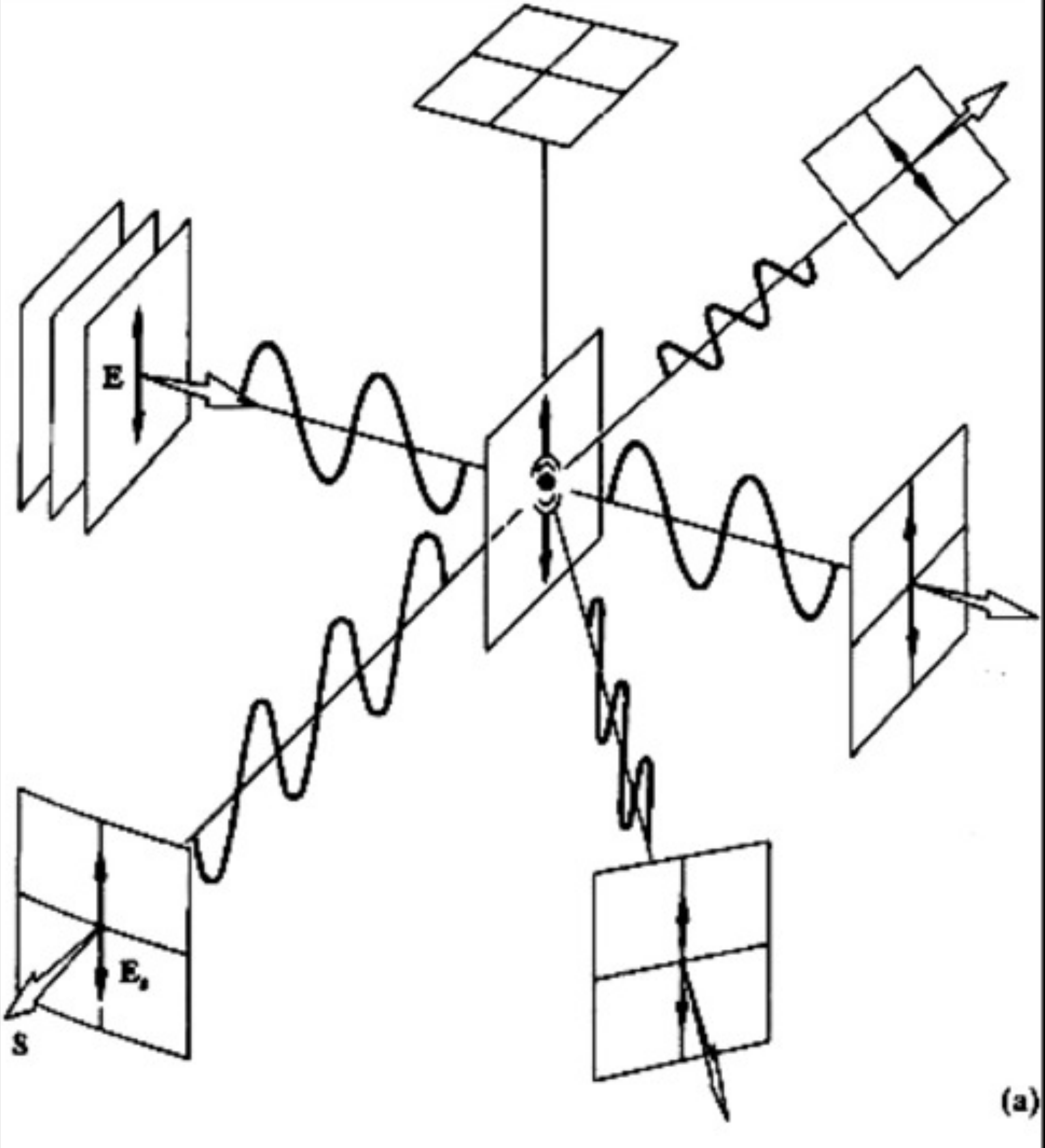


FIGURE 8.35a Scattering of polarized light by a molecule.

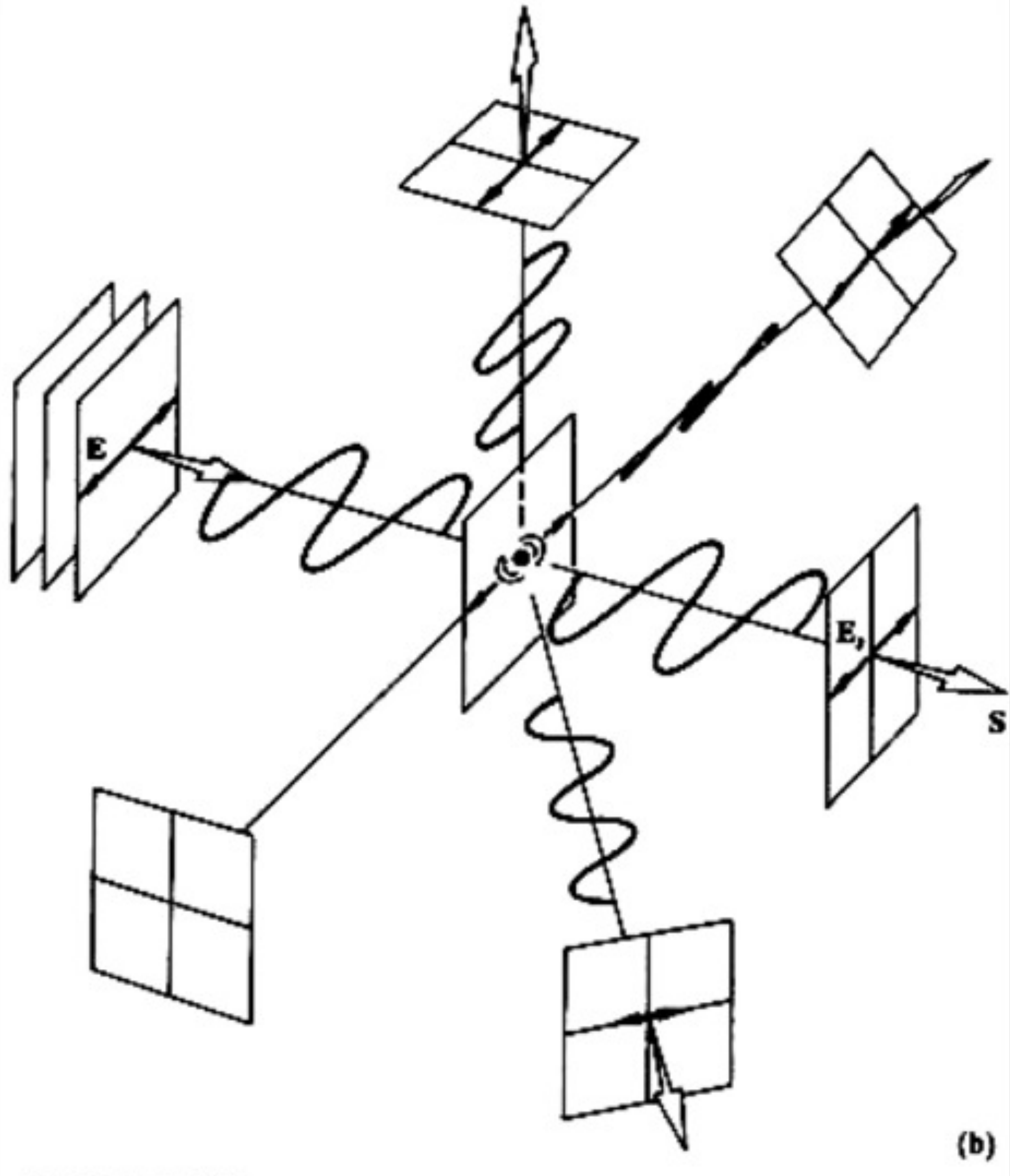
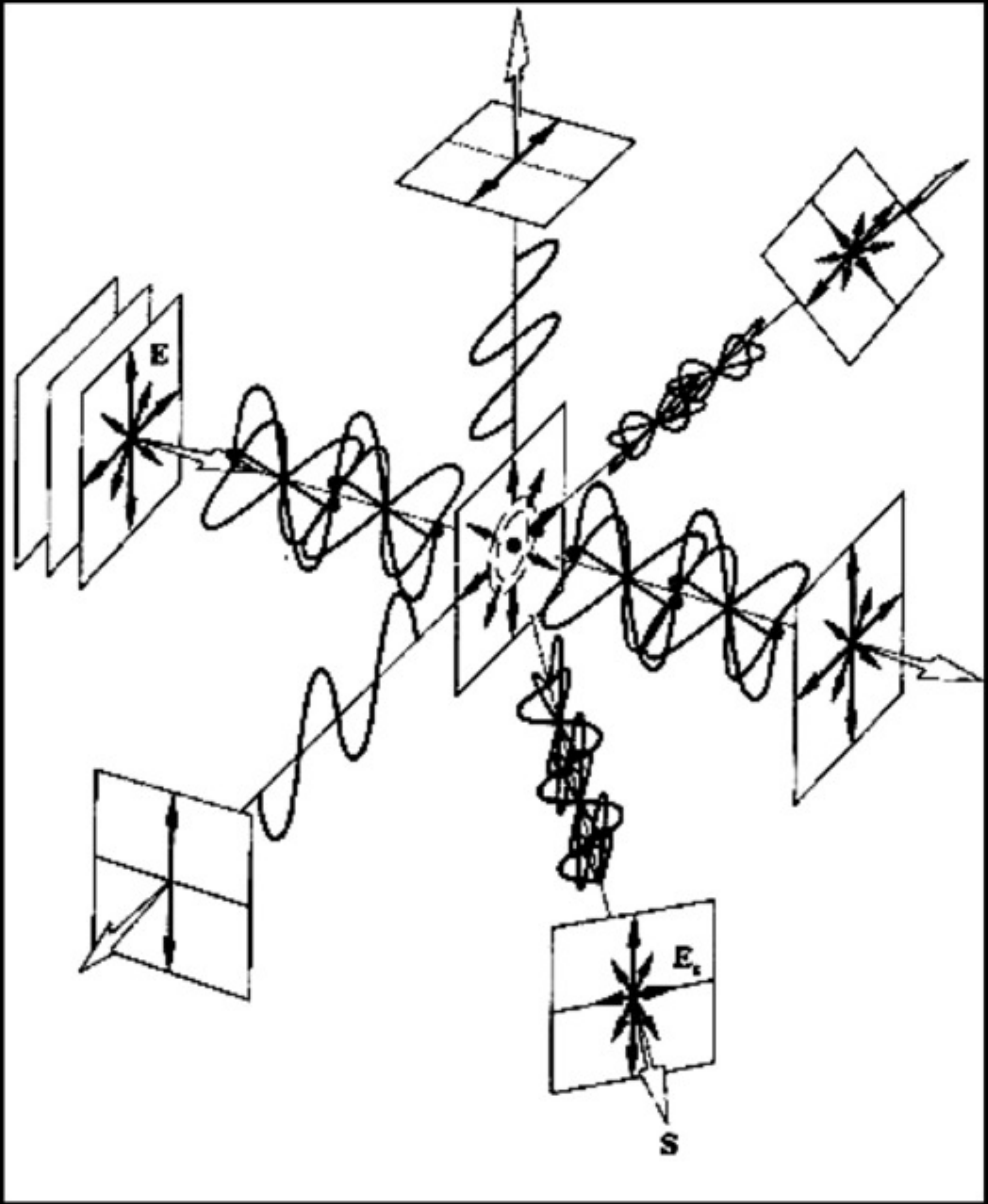


FIGURE 8.35b

http://www.physics.gatech.edu/MOPED/Theory/PbS_files/image002.jpg

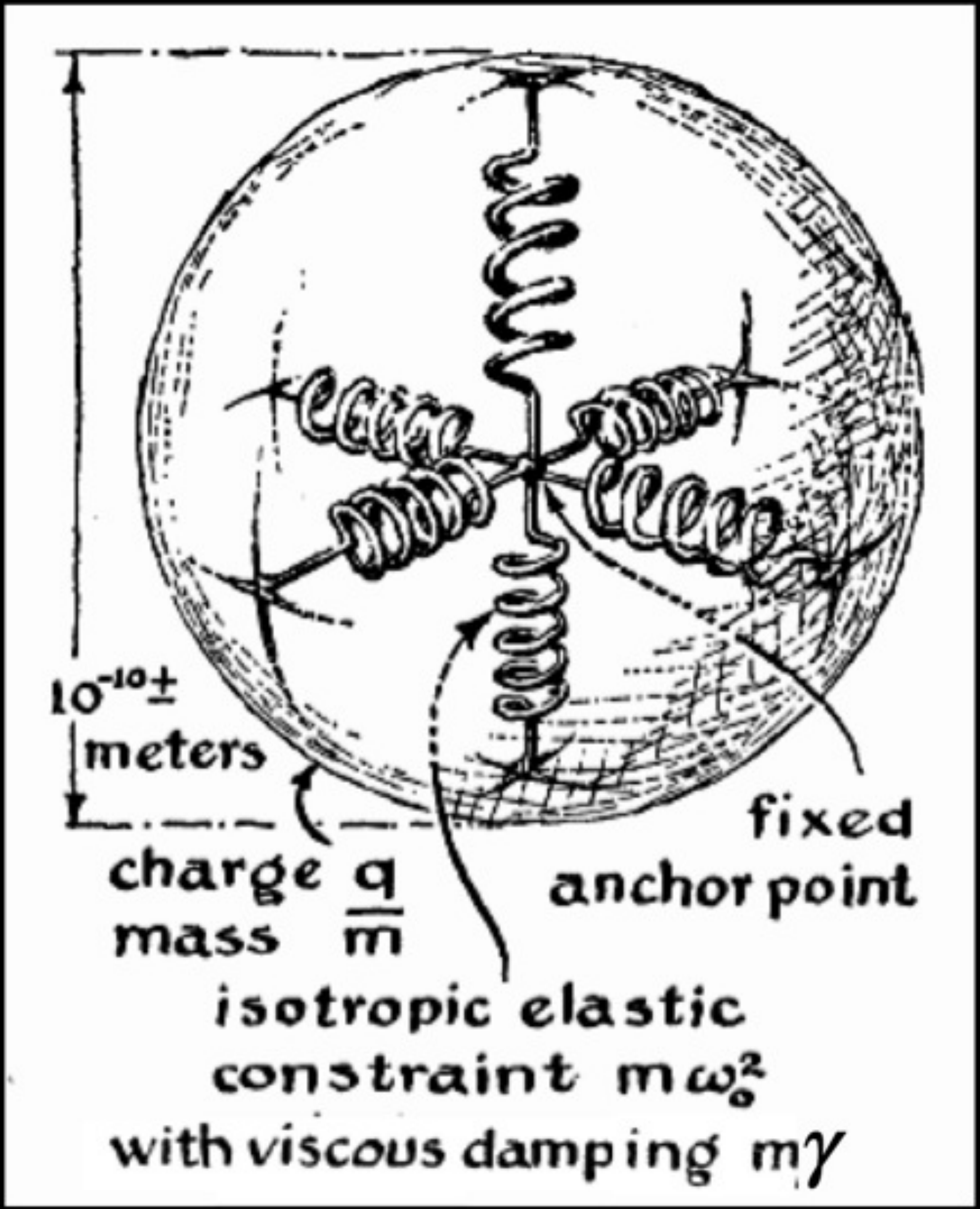
Scattering of unpolarized em radiation

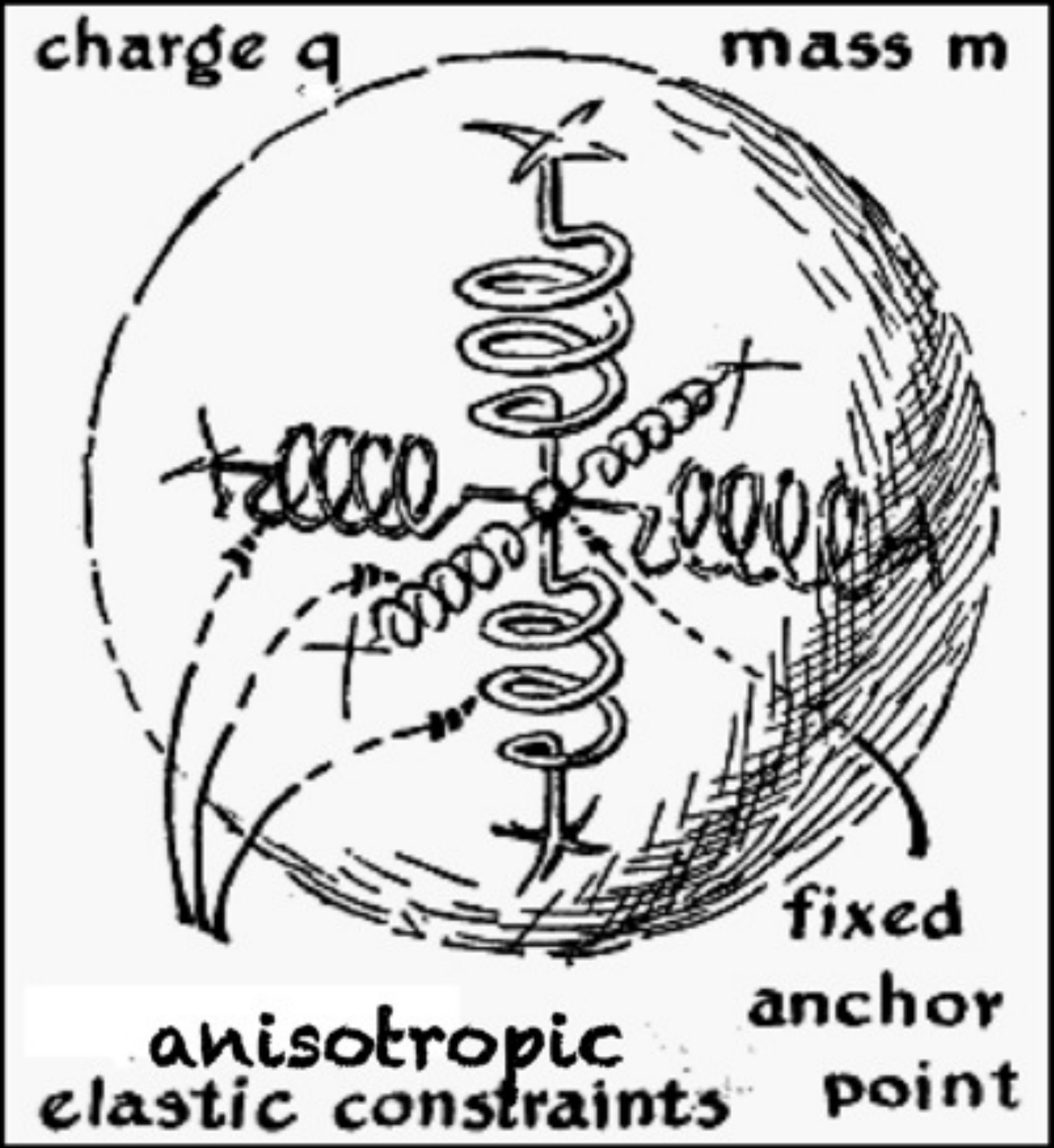


http://www.physics.gatech.edu/MOPED/Theory/PbS_files/image006.jpg

Mechanical models for electron oscillators

Spheres of uniform charge density with total charge *q* and mass *m*





Classical electron radius

Electrostatic potential energy

$$E = q\phi(r) = q(q/r) = e^2/r_e$$

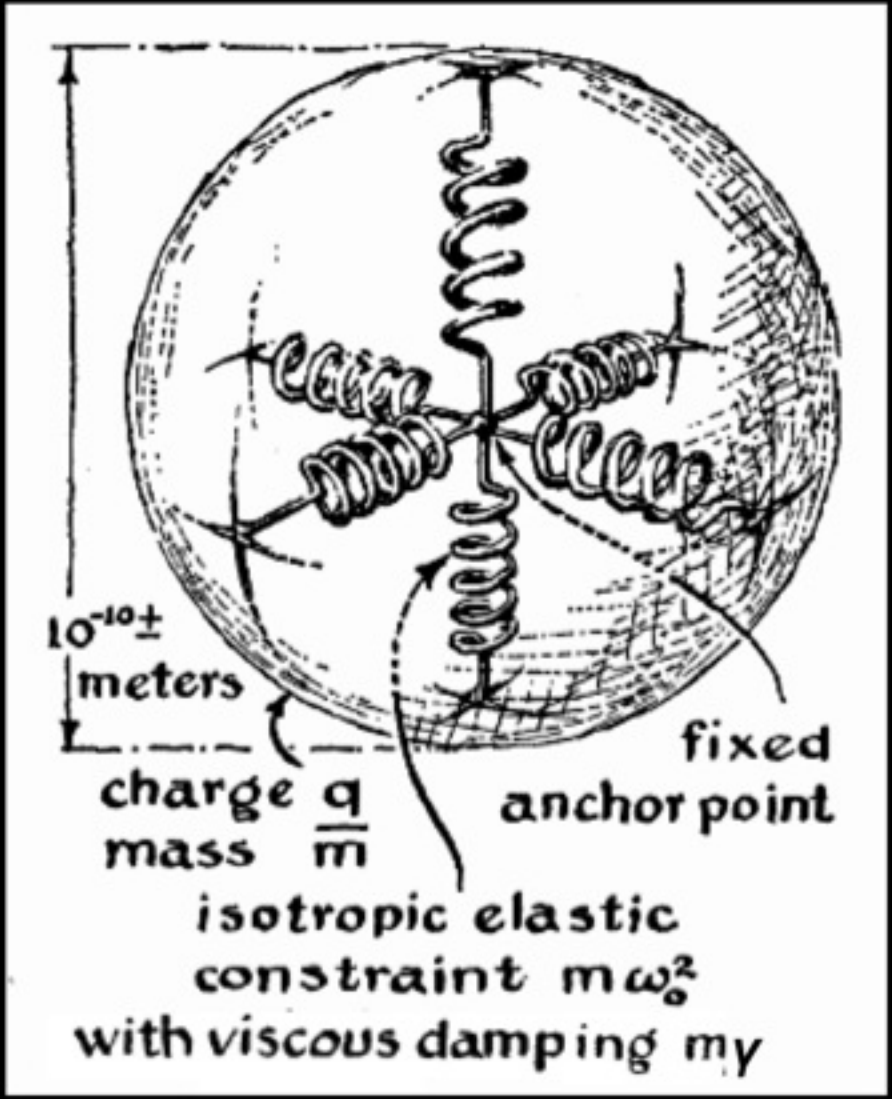
Relativistic mass - energy

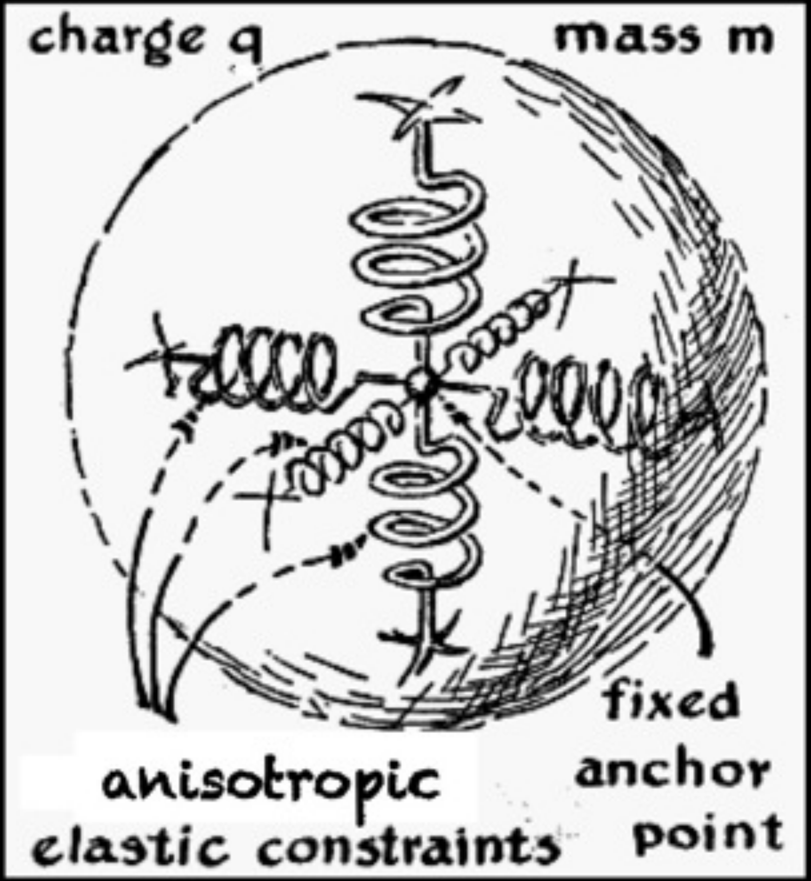
$$E = m_e c^2$$

$$\left.\right\} \quad r_e = \frac{e^2}{m_e c^2}$$

John Strong (1958). *Concepts of Classical Optics*. San Francisco: W.H. Freeman & Co.

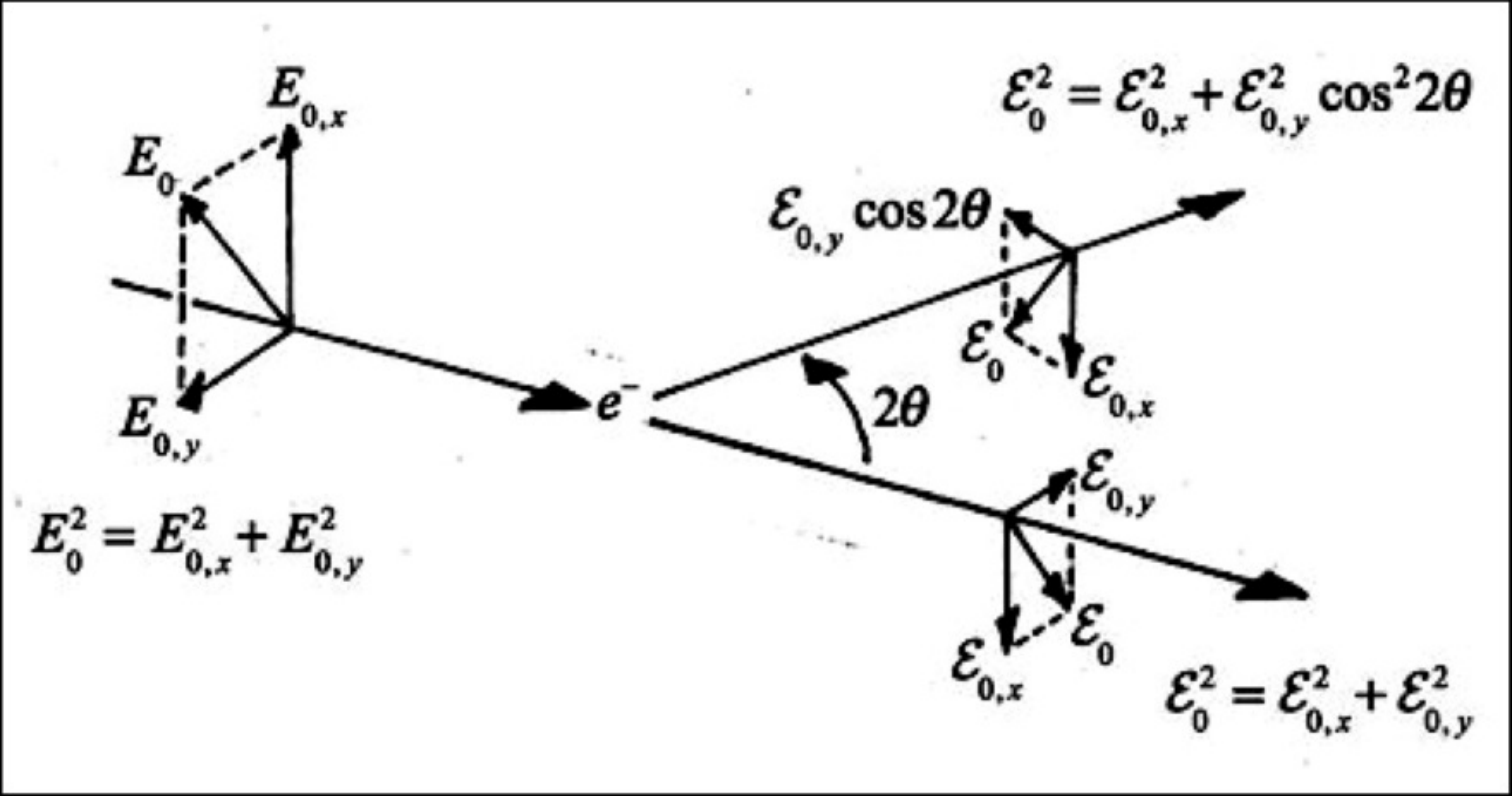
Mechanical models for 3-D oscillators





If a electron is driven to oscillate by an ***unpolarized* em *wave***, the electron oscillations will be ***three dimensional***.

Scattering of a linearly polarized beam with an arbitrary direction of polarization



Diffracted X-ray beam polarization

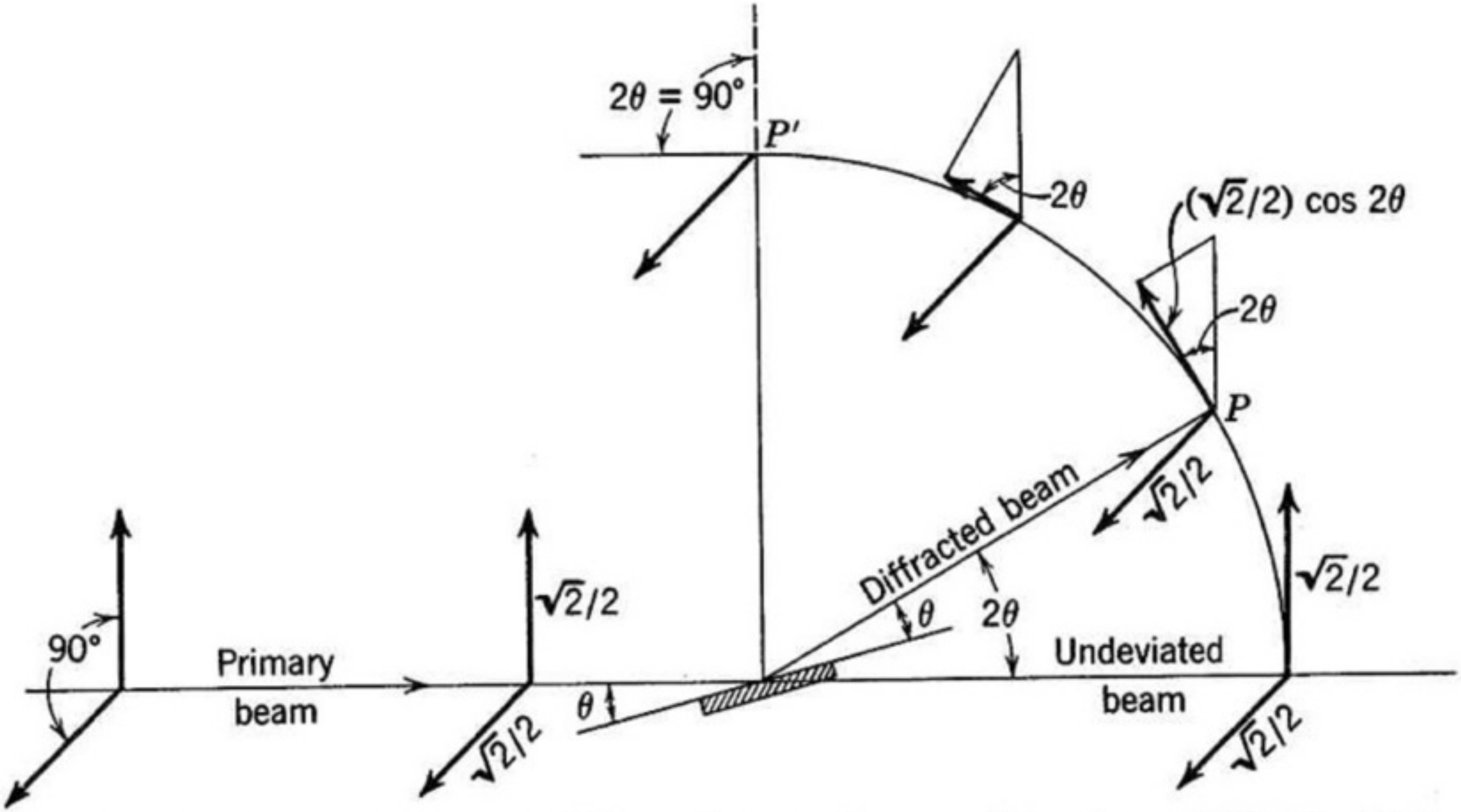


Fig. 3–11. Polarization of a diffracted x-ray beam. (Courtesy of Blake, *Revs. Mod. Phys.*, 5, 169.)

Any vector of unit length can be resolved into a pair of perpendicular components each of length $\sqrt{2}/2$.
The component perpendicular to the equatorial plane of the incident and diffracted beams remains constant;
the in-plane component varies as cos $\left(\sqrt{2}/2\right)$

Harold P. Klug and Leroy E. Alexander (1954). *X-Ray Diffraction Procedures for Polycrystalline and Amorphous Materials*. New York: John Wiley.

X-ray scattering by a bound electron in a free atom

(Gaussian cgs units)

$$m\frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = -e\mathbf{E}_0\mathrm{e}^{i\omega t} \quad -k\mathbf{x} \quad , \qquad k = m\omega_0^2 \quad \text{elastic force constant}$$

Newton's second law force
F=*m*a

em Coulombic driving force
F=*q*E

Hooke's law elastic restoring force
F=−*k*x

$$\begin{cases} \mathbf{x} = \mathbf{x}_0\mathrm{e}^{i\omega t}, \qquad \mathbf{v} = \dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = i\,\omega\mathbf{x}_0\mathrm{e}^{i\omega t}, \qquad \mathbf{a} = \dfrac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \dfrac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = -\omega^2\mathbf{x}_0\mathrm{e}^{i\omega t} \\ -m\,\omega^2\mathbf{x}_0\mathrm{e}^{i\omega t} = -e\mathbf{E}_0\mathrm{e}^{i\omega t} - k\mathbf{x}_0\mathrm{e}^{i\omega t} \\ \qquad m\omega^2\mathbf{x} = e\mathbf{E} + k\mathbf{x} \end{cases}$$

$$\mathbf{x} = \frac{e\mathbf{E}}{m\omega^2 - k} = \frac{e\mathbf{E}}{m\left(\omega^2 - \dfrac{k}{m}\right)} = \frac{e\mathbf{E}_0}{m}\left(\frac{1}{\omega^2 - \omega_0^2}\right)\mathrm{e}^{i\omega t}, \qquad \omega_0 = \sqrt{k/m}$$

$$\mathbf{a} = -\omega^2\mathbf{x} = -\frac{e\mathbf{E}}{m}\left(\frac{\omega^2}{\omega^2 - \omega_0^2}\right)$$

$$\mathcal{E} = -\frac{q\,\mathbf{a}}{c^2 r} = -\left(\frac{-e}{c^2 r}\right)\frac{e\mathbf{E}}{m}\left(\frac{\omega^2}{\omega^2 - \omega_0^2}\right)\mathrm{e}^{i\omega t} = \underbrace{\underbrace{\left(\frac{e^2}{mc^2}\right)}_{r_\mathrm{e}}\frac{\mathbf{E}_0}{r}}_{\mathcal{E}_0}\left(\frac{\omega^2}{\omega^2 - \omega_0^2}\right)\mathrm{e}^{i\omega t} = \mathcal{E}_0\mathrm{e}^{i\omega t}$$

Resonant X-ray scattering by a bound atomic electron

(Gaussian cgs units)

damped driven harmonic oscillator

$$m\frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = -\kappa\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \quad -k\,\mathbf{x} \quad -e\mathbf{E}_0\,\mathrm{e}^{i\omega t}\,, \qquad \begin{cases} k = m\omega_0^2 & \text{nucleus-electron elastic force constant} \\ \kappa = m\gamma & \text{radiation loss damping force constant} \end{cases}$$

Newton's second law force F=*m*a

radiation loss damping force F=−κv

Hooke's law restoring force F=−*k*x

Coulombic em driving force F=*q*E

$$\mathbf{x} = \mathbf{x}_0\,\mathrm{e}^{i\omega t}, \qquad \mathbf{x}_0 = \frac{e\mathbf{E}_0}{m}\left(\frac{1}{\omega^2 - \omega_0^2 - i\gamma\omega}\right)$$

$$\mathbf{a} = \frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = -\omega^2\mathbf{x}_0\,\mathrm{e}^{i\omega t} = \mathbf{a}_0\,\mathrm{e}^{i\omega t}, \qquad \mathbf{a}_0 = -\omega^2\mathbf{x}_0 = -\frac{e\mathbf{E}_0}{m}\left(\frac{\omega^2}{\omega^2 - \omega_0^2 - i\gamma\omega}\right)$$

$$\mathcal{E}_0 = -\frac{q\,\mathbf{a}_0}{c^2 r} = -\underbrace{\underbrace{\left(\frac{e^2}{m_\mathrm{e}c^2}\right)\frac{\mathbf{E}_0}{r}}_{\text{free } e^- \text{ scattered X-ray wave amplitude at } \mathbf{r}}\left(\frac{\omega^2}{\omega^2 - \omega_0^2 - i\gamma\omega}\right)}_{\text{bound } e^- \text{ scattered X-ray wave amplitude at } \mathbf{r}}$$

$$f_\mathrm{e} = \frac{\mathcal{E}_0(\text{bound})}{\mathcal{E}_0(\text{free})} = \frac{\omega^2}{\omega^2 - \omega_0^2 - i\gamma\omega} = \frac{1}{1 - \left(\frac{\omega_0}{\omega}\right)^2 - \frac{i\gamma}{\omega}}$$

X-ray scattering by a bound atomic electron is approximately the same as scattering by a free electron at rest (Gaussian cgs units)

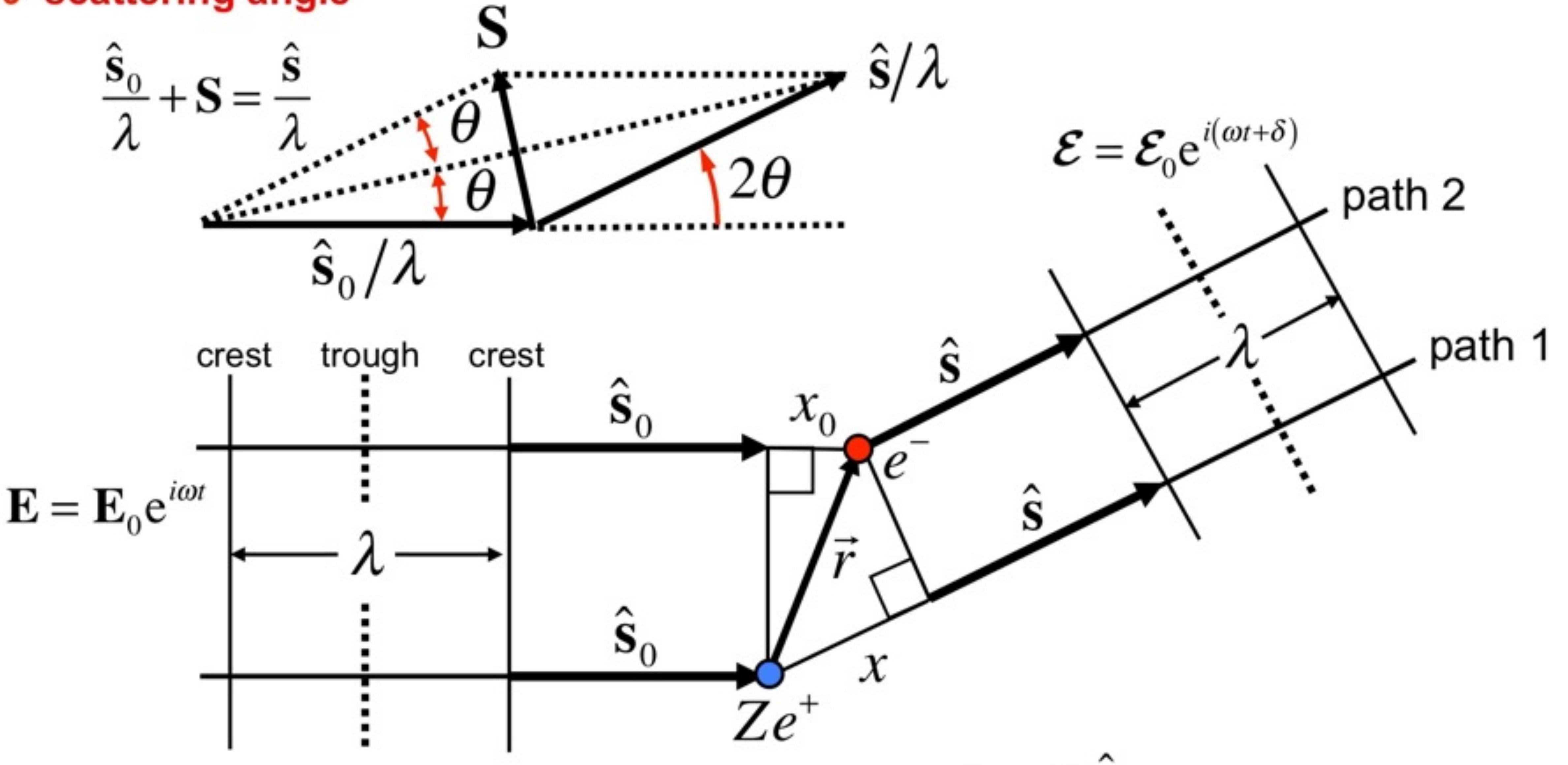
$$\mathcal{E}_0 = -\frac{q\,\mathbf{a}_0}{c^2 r} = \underbrace{\underbrace{-\left(\frac{e^2}{m_\mathrm{e} c^2}\right)\frac{\mathbf{E}_0}{r}}_{\substack{\text{free } e^- \text{ scattered} \\ \text{X-ray wave} \\ \text{amplitude at } \mathbf{r}}}\left(\frac{\omega^2}{\omega^2-\omega_0^2-i\gamma\omega}\right)}_{\substack{\text{bound } e^- \text{ scattered} \\ \text{X-ray wave} \\ \text{amplitude at } \mathbf{r}}}$$

$$f_\mathrm{e} = \frac{\mathcal{E}_0(\text{bound})}{\mathcal{E}_0(\text{free})} = \frac{\omega^2}{\omega^2-\omega_0^2-i\gamma\omega} = \frac{1}{1-\left(\dfrac{\omega_0}{\omega}\right)^2-\dfrac{i\gamma}{\omega}}$$

$$\left.\begin{array}{llll} \gamma \ll \omega & \Rightarrow & f_\mathrm{e} \approx \dfrac{1}{1-\left(\dfrac{\omega_0}{\omega}\right)^2} & \text{undamped oscillation} \\ \\ \omega_0 \ll \omega & \Rightarrow & f_\mathrm{e} \approx 1 & \text{high frequency limit} \end{array}\right\} \quad \text{free electron at rest} \quad f_\mathrm{e} = 1$$

X-ray scattering by an atomic electron

θ Bragg angle
2θ scattering angle



$$x_0 = \mathbf{r} \bullet \hat{\mathbf{s}}_0$$

$$x = \mathbf{r} \bullet \hat{\mathbf{s}}$$

$$|\hat{\mathbf{s}}_0| = |\hat{\mathbf{s}}| = 1$$

$$\hat{\mathbf{s}}_0 \bullet \hat{\mathbf{s}} = \cos 2\theta$$

$$\text{path } 1 = |\hat{\mathbf{s}}_0| + x + |\hat{\mathbf{s}}|$$

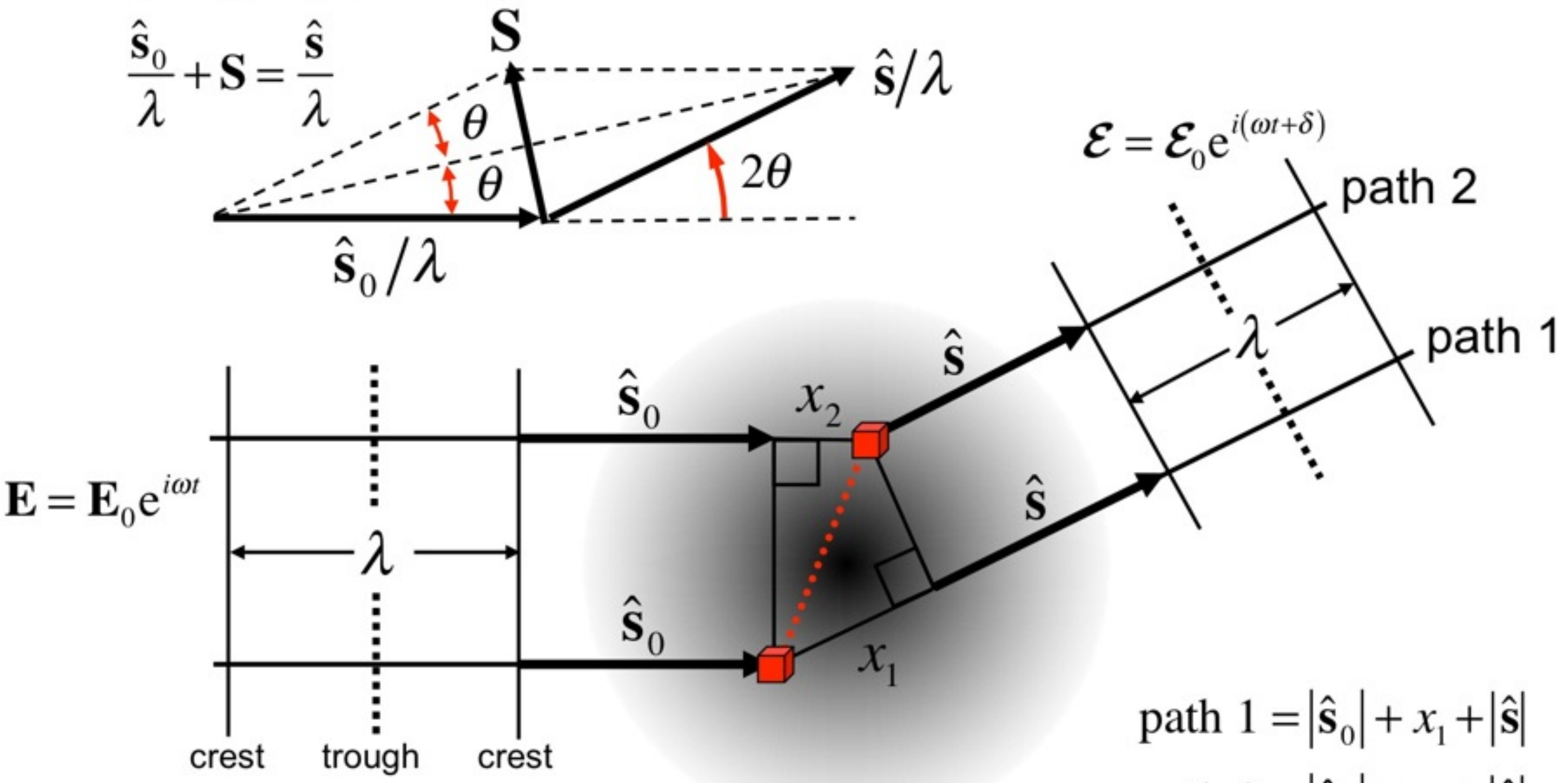
$$\mathbf{S} = \frac{\hat{\mathbf{s}} - \hat{\mathbf{s}}_0}{\lambda}, \qquad |\mathbf{S}| = 2\left(\frac{\sin\theta}{\lambda}\right)$$

$$\text{path } 2 = |\hat{\mathbf{s}}_0| + x_0 + |\hat{\mathbf{s}}|$$

$$\text{path } 1 - \text{path } 2 = x - x_0 = \mathbf{r} \bullet \hat{\mathbf{s}} - \mathbf{r} \bullet \hat{\mathbf{s}}_0 = \mathbf{r} \bullet (\hat{\mathbf{s}} - \hat{\mathbf{s}}_0)$$

X-ray scattering by different volume elements of an atomic electron density distribution

θ Bragg angle
2θ scattering angle



$$\frac{\hat{\mathbf{s}}_0}{\lambda} + \mathbf{S} = \frac{\hat{\mathbf{s}}}{\lambda}$$

$$\mathbf{E} = \mathbf{E}_0 e^{i\omega t}$$

$$\mathcal{E} = \mathcal{E}_0 e^{i(\omega t + \delta)}$$

$$\text{path } 1 = |\hat{\mathbf{s}}_0| + x_1 + |\hat{\mathbf{s}}|$$

$$\text{path } 2 = |\hat{\mathbf{s}}_0| + x_2 + |\hat{\mathbf{s}}|$$

$$\text{path } 2 - \text{path } 1 = x_2 - x_1 = \Delta x$$

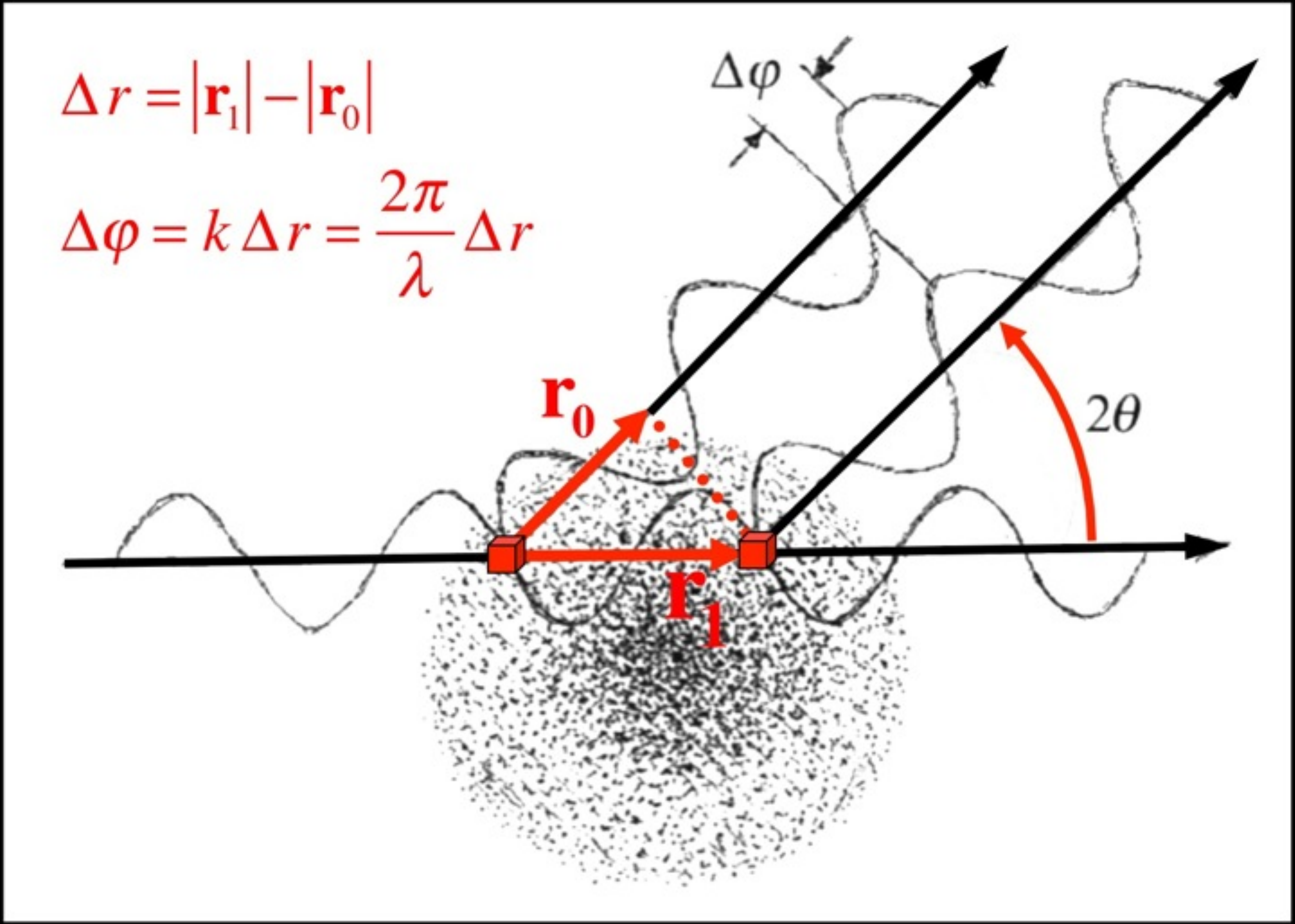
$$|\hat{\mathbf{s}}_0| = |\hat{\mathbf{s}}| = 1$$

$$\hat{\mathbf{s}}_0 \bullet \hat{\mathbf{s}} = \cos 2\theta$$

$$\mathbf{S} = \frac{\hat{\mathbf{s}} - \hat{\mathbf{s}}_0}{\lambda}, \qquad |\mathbf{S}| = 2\left(\frac{\sin\theta}{\lambda}\right)$$

$$\Delta\varphi = k\Delta x = \frac{2\pi}{\lambda}\Delta x$$

Phase differences due to scattering from different volume elements of an atomic electron density distribution



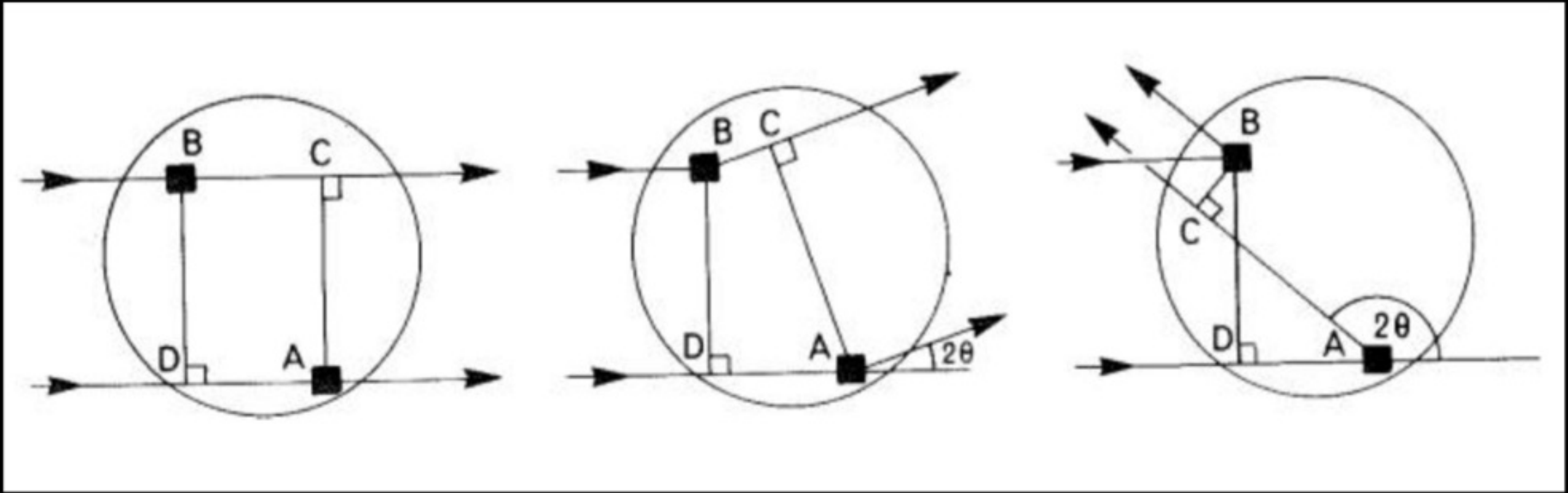
$$\Delta r = |\mathbf{r}_1| - |\mathbf{r}_0|$$

$$\Delta\varphi = k\,\Delta r = \frac{2\pi}{\lambda}\Delta r$$

Since X-ray wavelengths are comparable to atomic diameters, interference effects due to the differences in path lengths to and from each volume element of the atomic electron density distribution are responsible for the approximately Gaussian falloff of atomic scattering factors with increasing scattering angle.

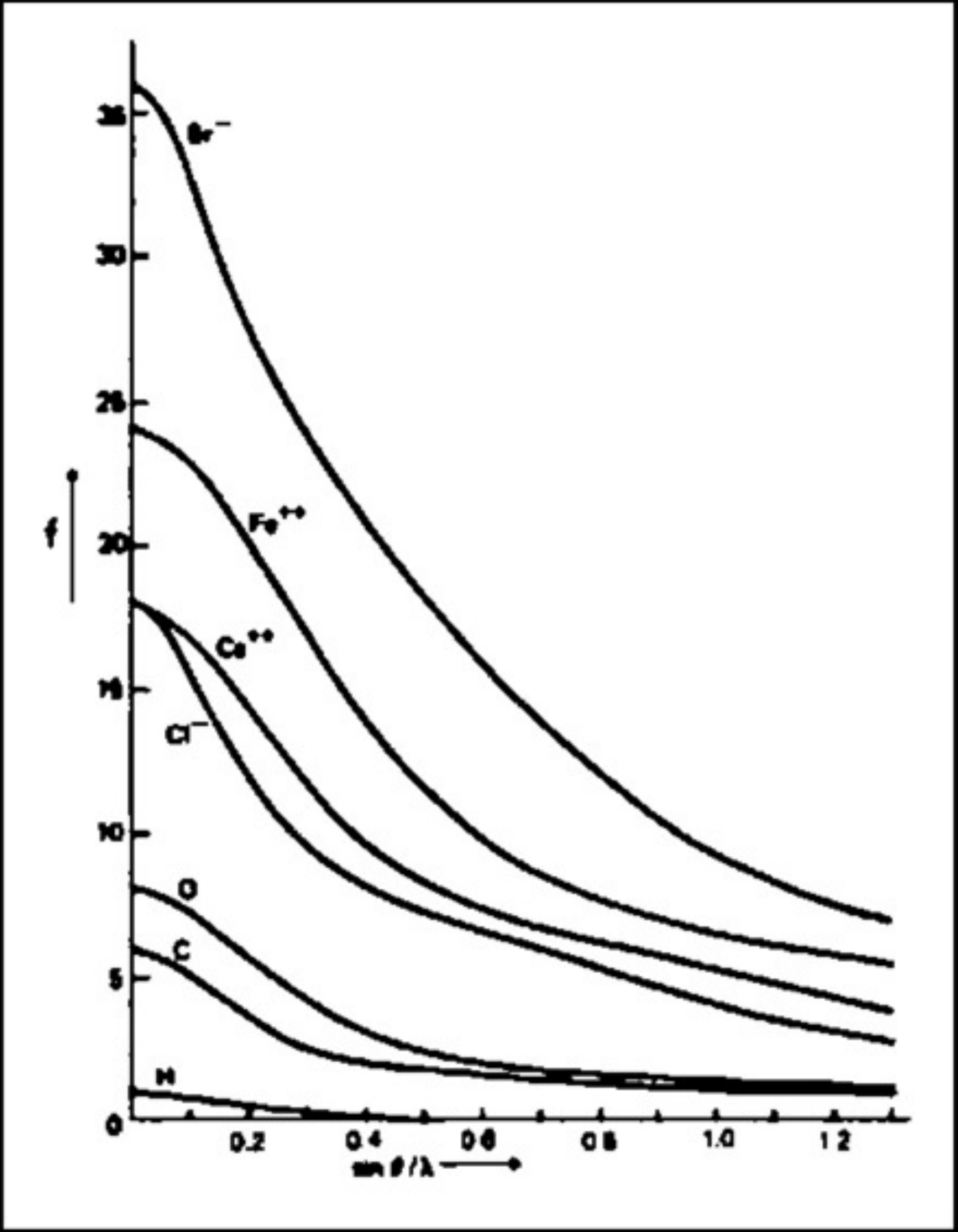
Figure adapted from Harold P. Klug and Leroy E. Alexander (1974). X-Ray Diffraction Procedures for Polycrystalline and Amorphous Materials. New York: John Wiley.

Scattering factor *versus* scattering angle



The higher the scattering angle,
the greater the difference between wave path lengths
the greater the destructive wave interference,
the greater the scattering factor fall-off with scattering angle

Scattering factor *versus* scattering angle



The atomic scattering factor $f_a(S)$ is roughly proportional to the atomic number Z_a.
At $S = (\sin \theta)/\lambda = 0$, $f_a(0) = Z_a$

http://www.xtal.iqfr.csic.es/Cristalografia/archivos_05/fac_scat3.jpg

Atomic Scattering Factors for X-rays

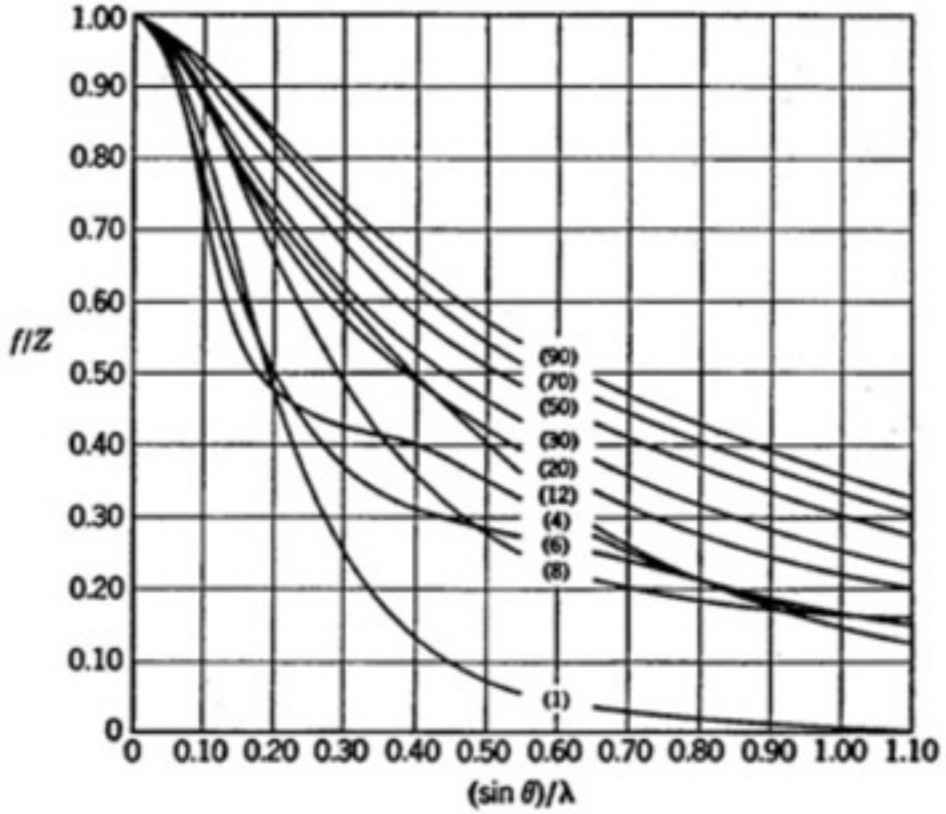


Fig. 20.

Variation of shapes of the curves of f/Z against $(\sin\theta)/\lambda$ for the chemical elements whose atomic numbers, Z, are given in parentheses. (After Harker and Kasper.[30])

Buerger (1960).

The "humps" or ripples in the f-curves for Z = 6 and Z = 4 occur because the $_4$Be $2s^2$ L-valence shell is filled and the $_6$C $2s^2 2p^2$ L-valence shell is half-filled. When a valence shell is filled or half-filled there is a slight real-space expansion of the outer, valence-shell electron density $\rho_v(r)$ and therefore a reciprocal-space contraction of the low-angle, valence-shell scattering factor curve $f_v(S) = \mathcal{F}^{-1}\left[\rho_v(r)\right]$.

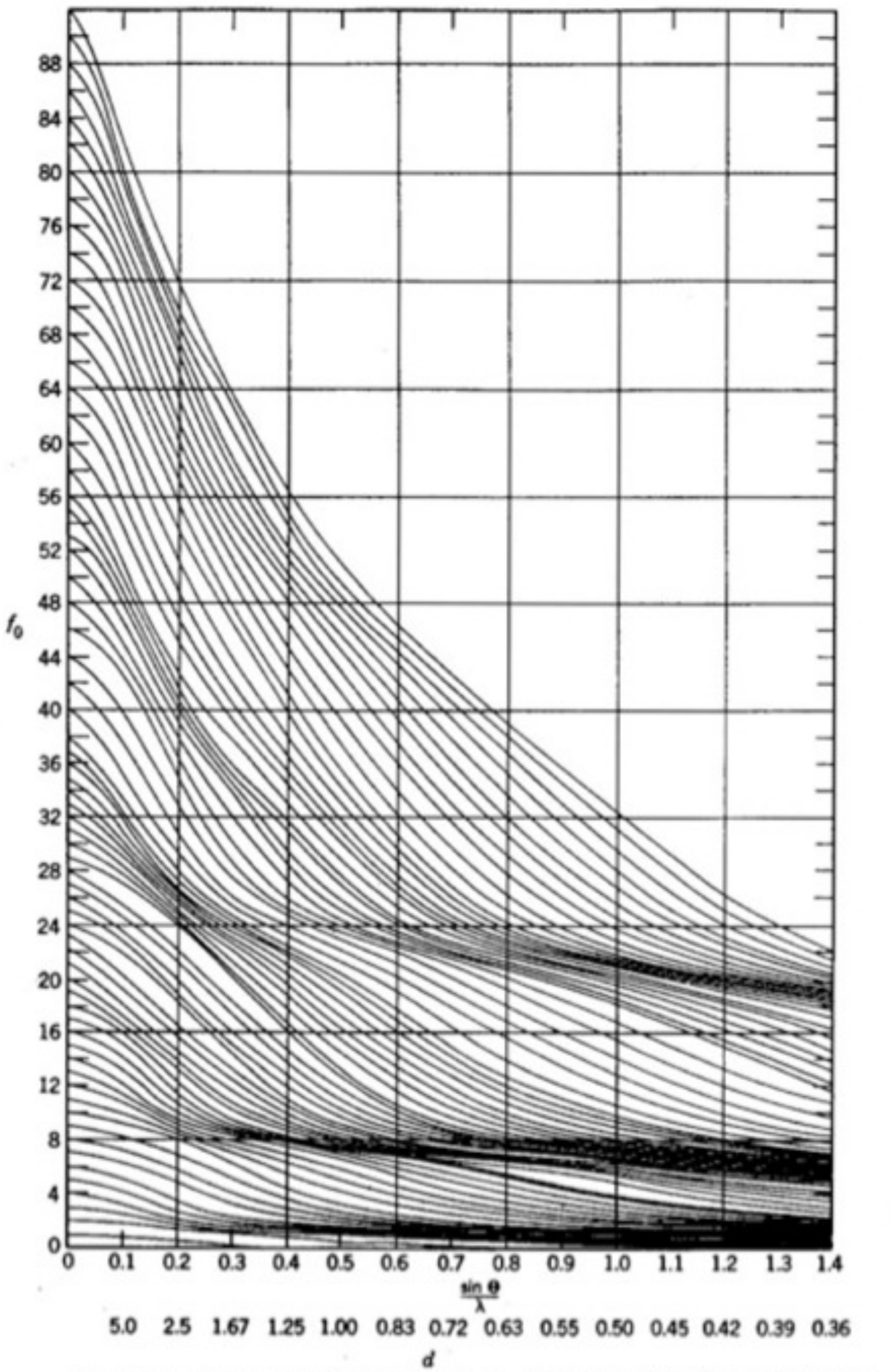
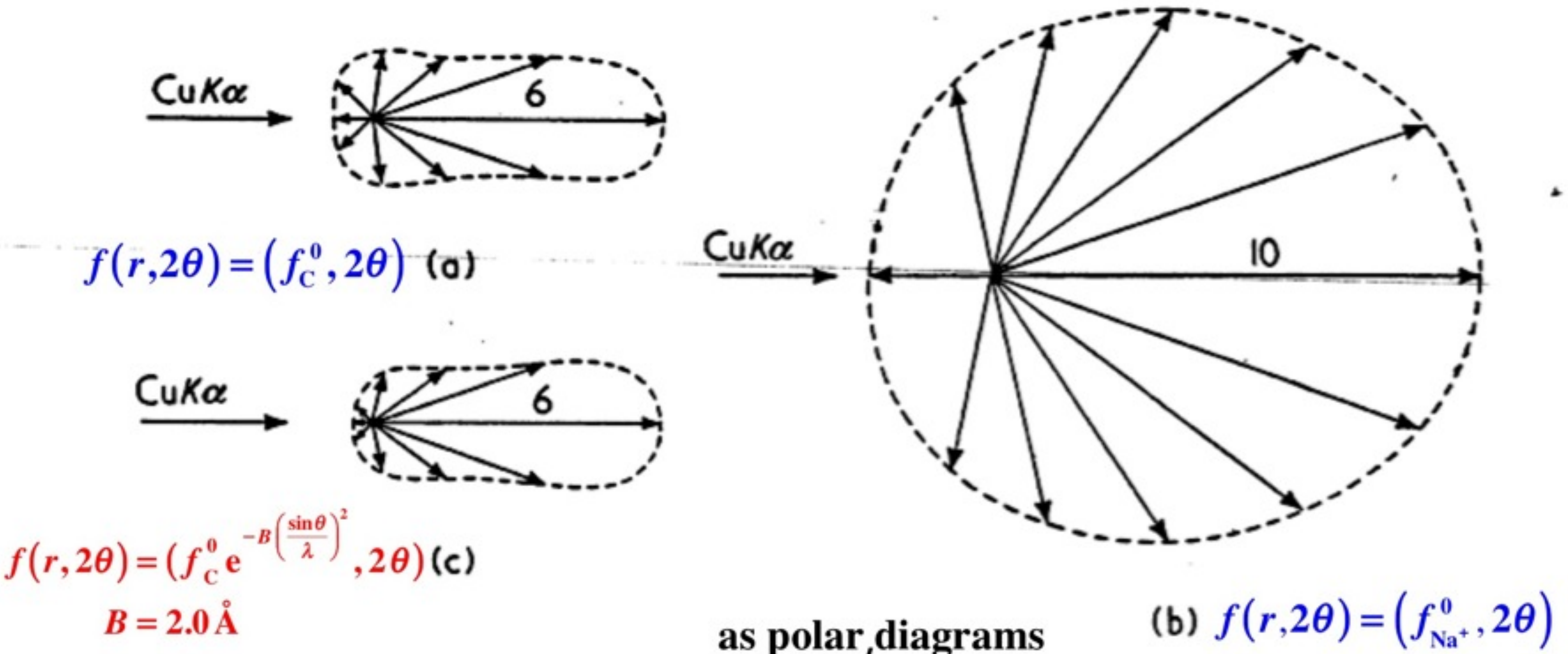


Fig. 3–13. Values of f_0 for neutral atoms. (Courtesy of Pauling and Sherman, *Z. Krist.*, *81*, 1.)

Klug & Alexander (1974).

Polar Plots of Atomic X-ray Scattering Factors versus scattering angle



$f(r,2\theta) = \left(f_{\mathrm{C}}^{0}, 2\theta\right)$ (a)

$f(r,2\theta) = (f_{\mathrm{C}}^{0} \mathrm{e}^{-B\left(\frac{\sin\theta}{\lambda}\right)^{2}}, 2\theta)$ (c)

$B = 2.0\,\text{Å}$

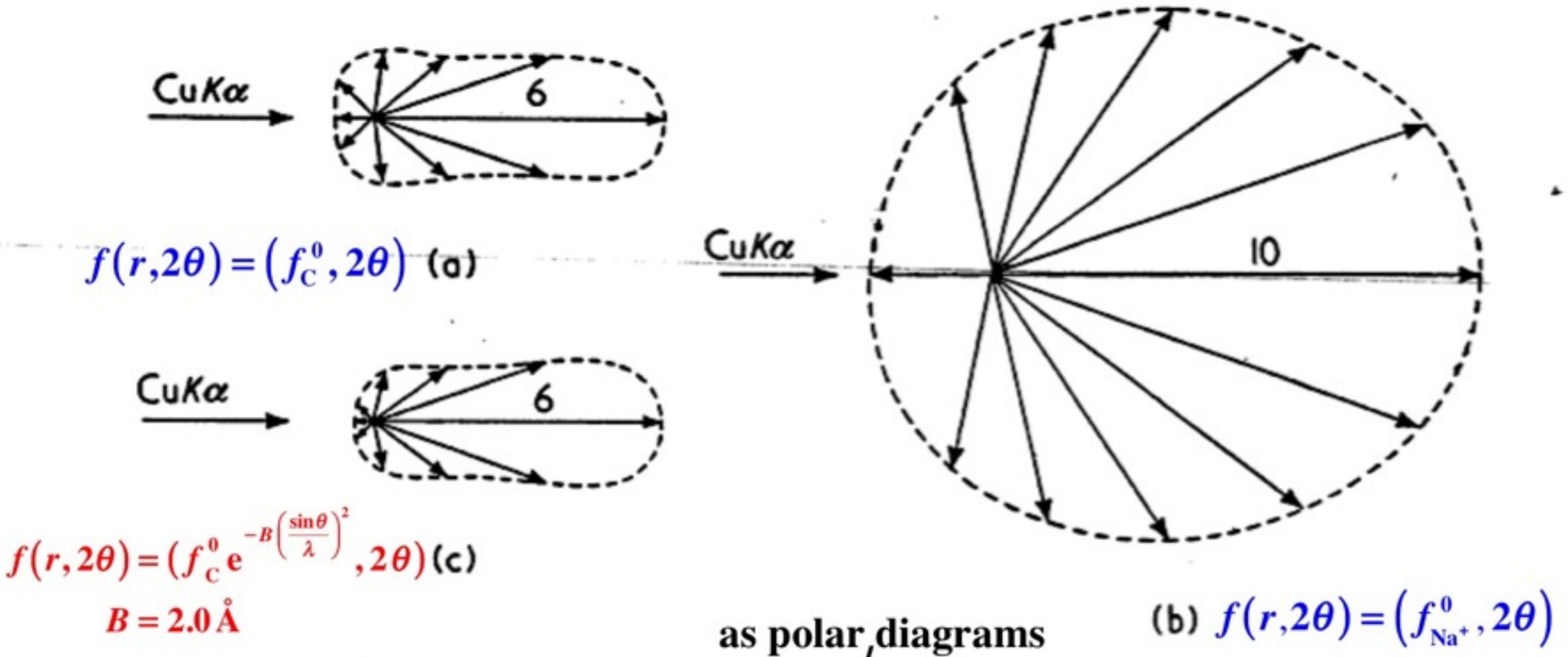
(b) $f(r,2\theta) = \left(f_{\mathrm{Na^{+}}}^{0}, 2\theta\right)$

Fig. 4.3. Scattering amplitudes (factors) as polar diagrams for (a) stationary carbon atom, (b) stationary sodium ion and (c) vibrating carbon atom, $B = 2{\cdot}0$ Å².

Due to interference effects among waves scattered from different volume elements of the atomic electron density distribution, the amplitude of scattering decreases with increasing scattering angle.

S.C. Nyburg (1961). X-Ray Analysis of Organic Structures. New York: Academic Press.

Polar Plots of Atomic X-ray Scattering Factors versus scattering angle



$f(r,2\theta)=\left(f_{\mathrm{C}}^{0},2\theta\right)$ (a)

$f(r,2\theta)=(f_{\mathrm{C}}^{0}\mathrm{e}^{-B\left(\frac{\sin\theta}{\lambda}\right)^{2}},2\theta)$ (c)

$B = 2.0\,\text{Å}$

(b) $f(r,2\theta)=\left(f_{\mathrm{Na^+}}^{0},2\theta\right)$

Fig. 4.3. Scattering amplitudes (factors) as polar diagrams for (a) stationary carbon atom, (b) stationary sodium ion and (c) vibrating carbon atom, $B = 2{\cdot}0$ Å².

Due to interference effects among waves scattered from different volume elements of the atomic electron density distribution, the amplitude of scattering decreases with increasing scattering angle.

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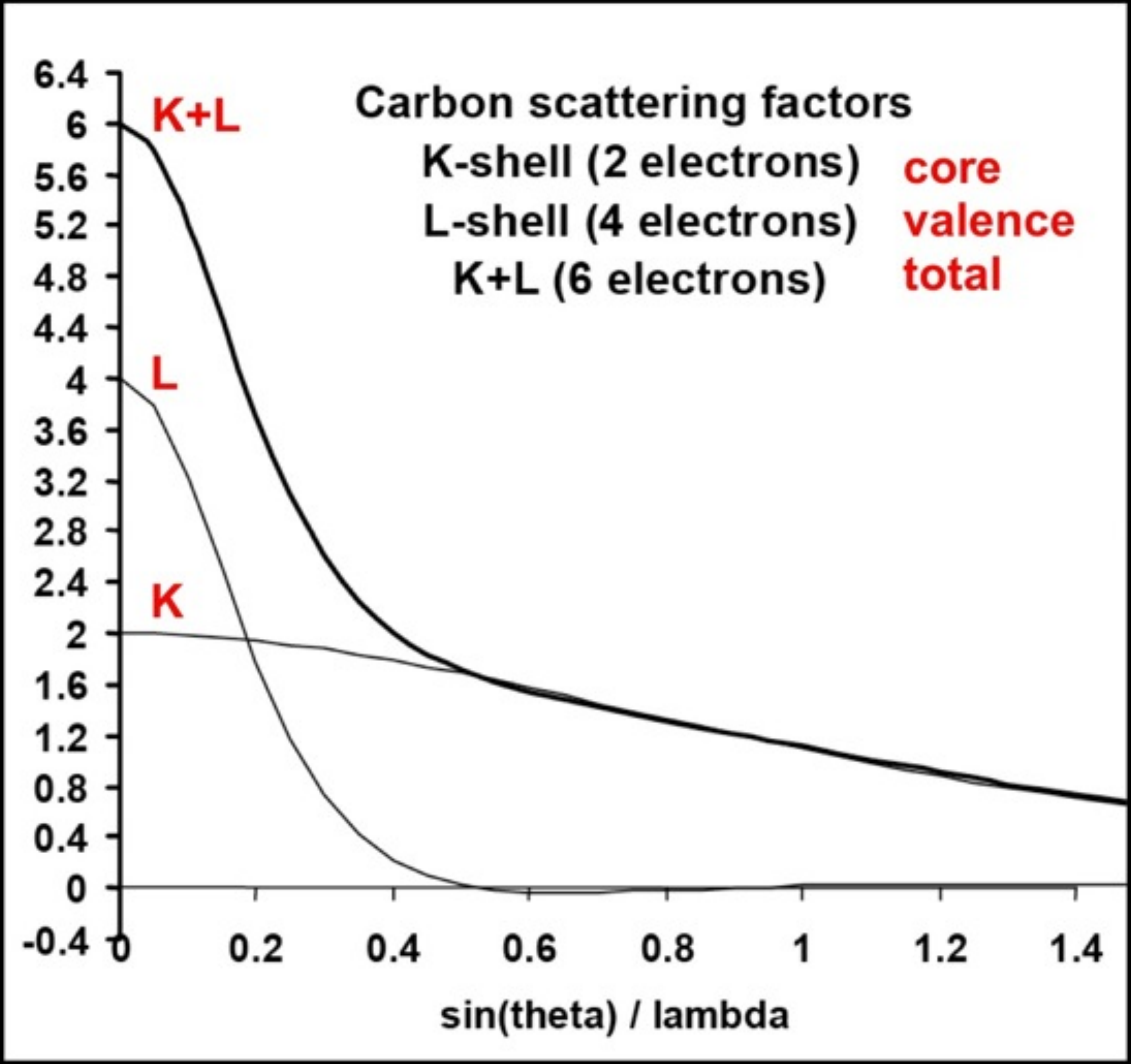
Carbon atom scattering from different electron shells



For carbon, the four-electron valence shell (L-shell) scattering is negligible for (sin $\theta)/\lambda$ > 0.5 Å^{-1}, d_{min} < 1 Å .

The two-electron inner shell (K-shell) scattering extends well beyond (sin $\theta)/\lambda$ = 1.4 Å^{-1} , d_{min} < 0.36 Å .

Radial electron density and scattering factor curves for K$^+$ [Ar] $1s^2 2s^2 2p^6 3s^2 3p^6$ subshells

$U(r) = 4\pi r^2 \left|R(r)\right|^2$ subshell curves

$f(S) = \int_0^\infty U(r) \frac{\sin(2\pi Sr)}{2\pi Sr} \mathrm{d}r$ subshell curves

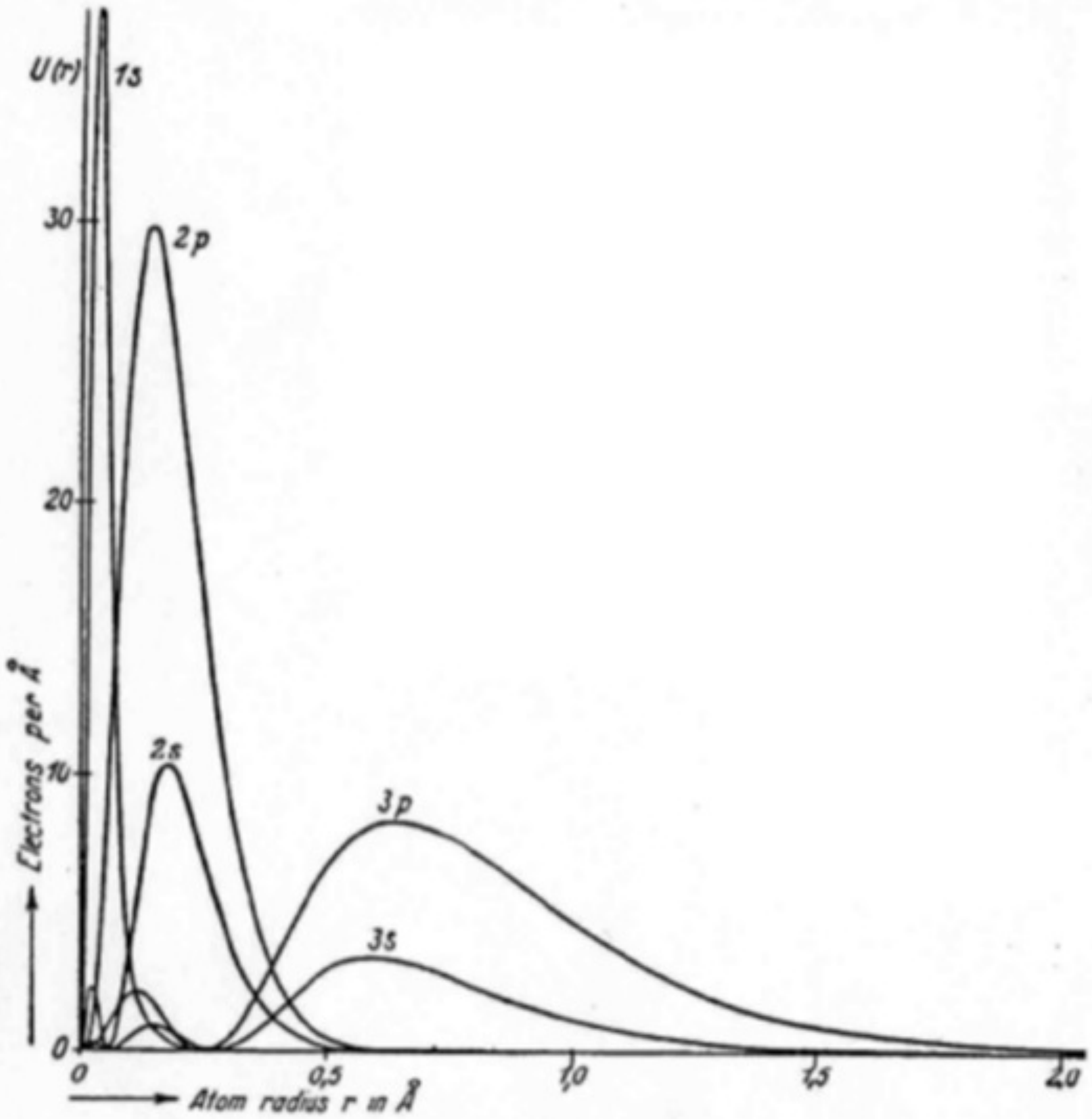


FIG. 43. Radial charge distribution for the different electron groups of K+
(James, *Ergebnisse der technischen Röntgenkunde*, vol. III, 1933)

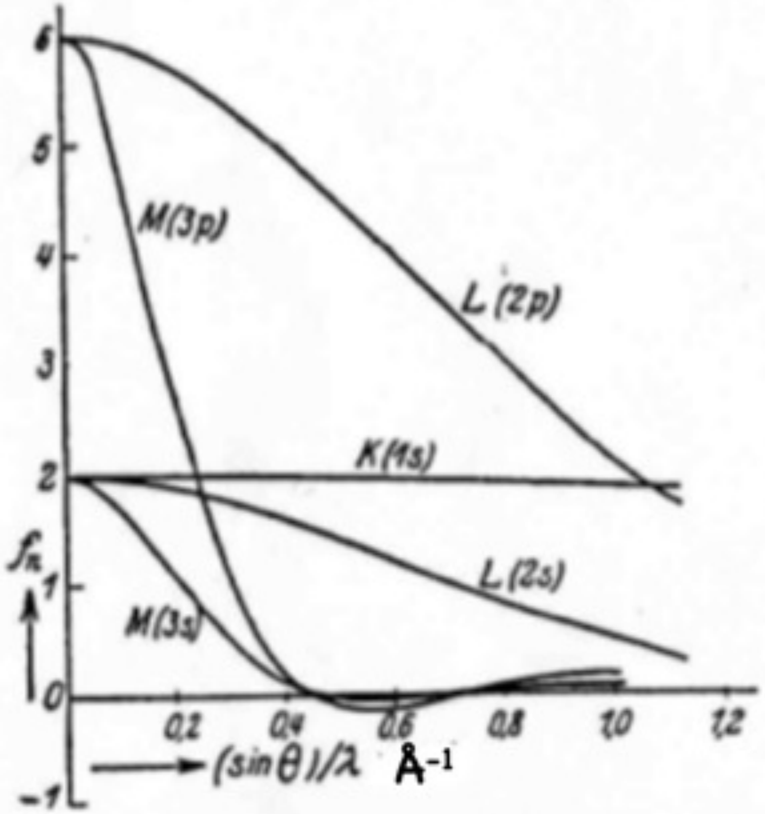


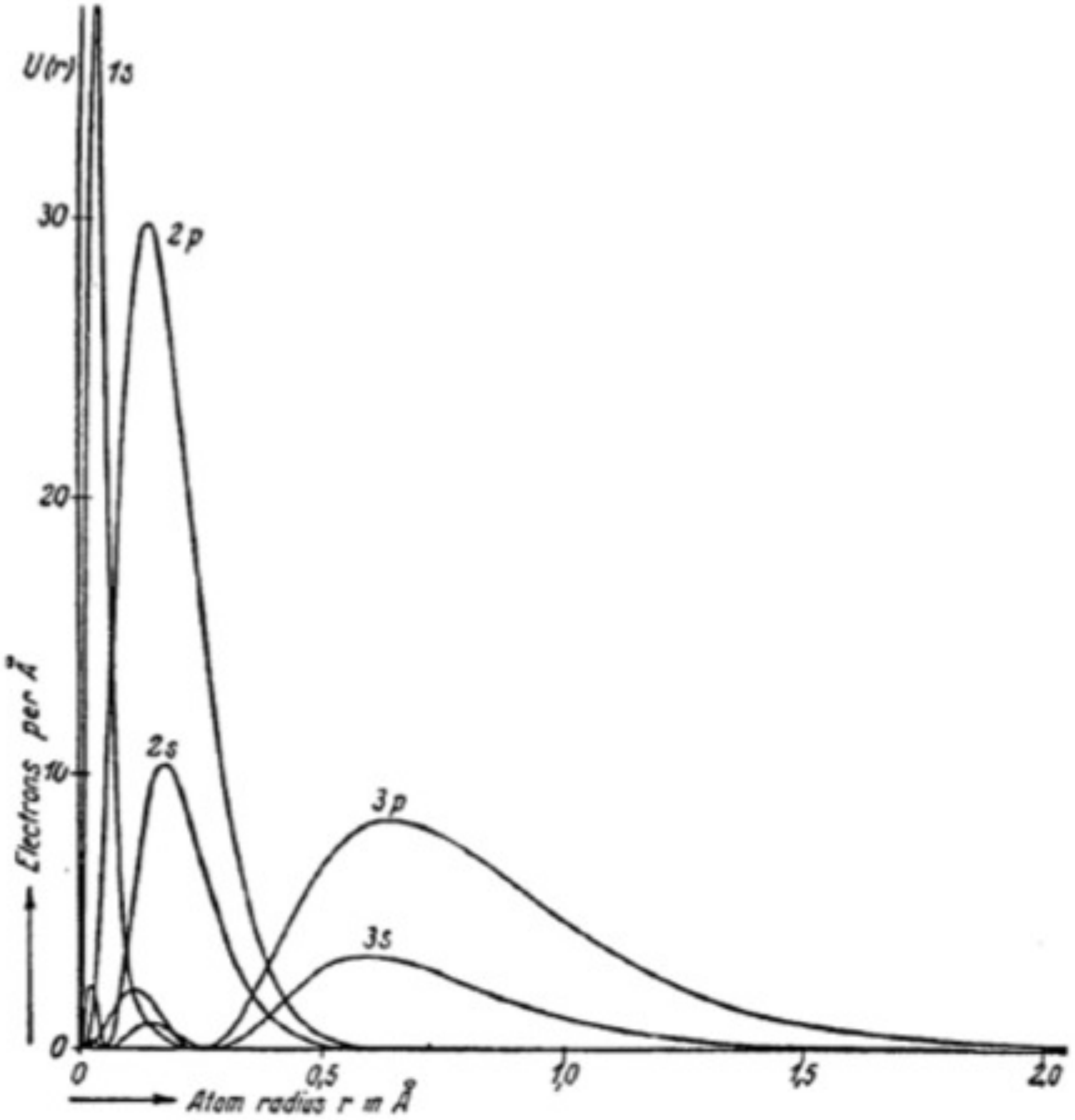
FIG. 48. *f*-curves for the individual electron groups of K+
(James, *Ergebnisse der technischen Röntgenkunde*, vol. III, 1933)

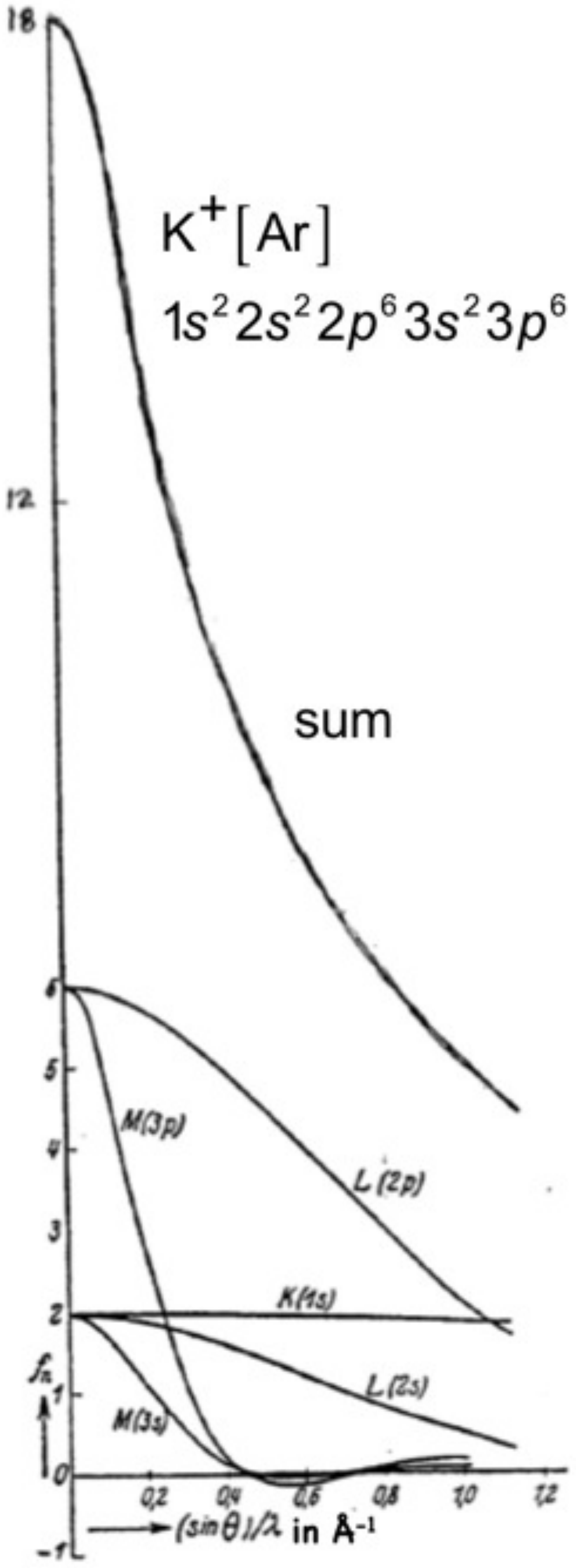
Figures copied from R.W. James, (1982). The *Optical Principles of the Diffraction of X-Rays.* Woodbridge, Connecticut: Ox Bow Press.

Radial electron density and scattering factor curves

$$f(S) = \mathcal{F}^{-1}\left[\rho(r)\right]$$

$$\begin{cases} \rho(r) = 4\pi r^2 \left|R(r)\right|^2 \\ f(S) = \int_0^\infty \rho(r)\dfrac{\sin(2\pi Sr)}{2\pi Sr}\,\mathrm{d}r \end{cases}$$





Figures copied and adapted from James (1982).